U.S. DEPARTMENT OF COMMERCE
National Technical Information Service

PB-245 915

PHOTOCHEMICAL OXIDANT MODELING. VOLUME I - TECHNIQUES APPLICABLE TO HIGHWAY SYSTEM EVALUATION

GCA Corporation

PREPARED FOR
Environmental Protection Agency

April 1975

KEEP UP TO DATE

Between the time you ordered this report—which is only one of the hundreds of thousands in the NTIS information collection available to you—and the time you are reading this message, several *new* reports relevant to your interests probably have entered the collection.

Subscribe to the **Weekly Government Abstracts** series that will bring you summaries of new reports *as soon as they are received by NTIS* from the originators of the research. The WGA's are an NTIS weekly newsletter service covering the most recent research findings in 25 areas of industrial, technological, and sociological interest—invaluable information for executives and professionals who must keep up to date.

The executive and professional information service provided by NTIS in the **Weekly Government Abstracts** newsletters will give you thorough and comprehensive coverage of government-conducted or sponsored research activities. And you'll get this important information within two weeks of the time it's released by originating agencies.

WGA newsletters are computer produced and electronically photocomposed to slash the time gap between the release of a report and its availability. You can learn about technical innovations immediately—and use them in the most meaningful and productive ways possible for your organization. Please request NTIS-PR-205/PCW for more information.

The weekly newsletter series will keep you current. But *learn what you have missed in the past* by ordering a computer **NTISearch** of all the research reports in your area of interest, dating as far back as 1964, if you wish. Please request NTIS-PR-186/PCN for more information.

WRITE: Managing Editor
5285 Port Royal Road
Springfield, VA 22161

Keep Up To Date With SRIM

SRIM (Selected Research in Microfiche) provides you with regular, automatic distribution of the complete texts of NTIS research reports *only* in the subject areas you select. SRIM covers almost all Government research reports by subject area and/or the originating Federal or local government agency. You may subscribe by any category or subcategory of our WGA **(Weekly Government Abstracts)** or **Government Reports Announcements and Index** categories, or to the reports issued by a particular agency such as the Department of Defense, Federal Energy Administration, or Environmental Protection Agency. Other options that will give you greater selectivity are available on request.

The cost of SRIM service is only 45¢ domestic (60¢ foreign) for each complete microfiched report. Your SRIM service begins as soon as your order is received and processed and you will receive biweekly shipments thereafter. If you wish, your service will be backdated to furnish you microfiche of reports issued earlier.

Because of contractual arrangements with several Special Technology Groups, not all NTIS reports are distributed in the SRIM program. You will receive a notice in your microfiche shipments identifying the exceptionally priced reports not available through SRIM.

A deposit account with NTIS is required before this service can be initiated. If you have specific questions concerning this service, please call (703) 451-1558, or write NTIS, attention SRIM Product Manager.

This information product distributed by

NTIS U.S. DEPARTMENT OF COMMERCE
National Technical Information Service
5285 Port Royal Road
Springfield, Virginia 22161

301023

PB 245 915

EPA-450/3-75-069-a
July 1975

PHOTOCHEMICAL OXIDANT MODELING

Volume I - Techniques Applicable to Highway System Evaluation

PRICES SUBJECT TO CHANGE

Reproduced by
NATIONAL TECHNICAL
INFORMATION SERVICE
US Department of Commerce
Springfield, VA. 22151

U.S. ENVIRONMENTAL PROTECTION AGENCY
Office of Air and Waste Management
Office of Air Quality Planning and Standards
Research Triangle Park, North Carolina 27711

EPA-450/3-75-069-a

PHOTOCHEMICAL OXIDANT MODELING Volume I - Techniques Applicable to Highway System Evaluation

by

F. A. Record, R. M. Patterson, D. A. Bryant, and A. H. Castaline

GCA Corporation
Bedford, Massachusetts 01730

Contract No. 68-02-1376, Task 14

EPA Project Officer: Thomas McCurdy

Prepared for

ENVIRONMENTAL PROTECTION AGENCY
Office of Air and Waste Management
Office of Air Quality Planning and Standards
Research Triangle Park, N. C. 27711

July 1975

iii

This report is issued by the Environmental Protection Agency to report technical data of interest to a limited number of readers. Copies are available free of charge to Federal employees, current contractors and grantees, and nonprofit organizations - as supplies permit - from the Air Pollution Technical Information Center, Environmental Protection Agency, Research Triangle Park, North Carolina 27711; or, for a fee, from the National Technical Information Service, 5285 Port Royal Road, Springfield, Virginia 22161.

This report was furnished to the Environmental Protection Agency by GCA Corporation, Bedford, Massachusetts 01730, in fulfillment of Contract No. 68-02-1376, Task 14. The contents of this report are reproduced herein as received from GCA Corporation. The opinions, findings, and conclusions expressed are those of the author and not necessarily those of the Environmental Protection Agency. Mention of company or product names is not to be considered as an endorsement by the Environmental Protection Agency.

Publication No. EPA-450/3-75-069-a

TECHNICAL REPORT DATA
(Please read Instructions on the reverse before completing)

1. REPORT NO. EPA-450/3-75-069-a	2.
3. RECIPIENT'S ACCESSION NO.	
4. TITLE AND SUBTITLE: Photochemical Oxidant Modeling: Volume I - Techniques Applicable to Highway System Evaluation.	5. REPORT DATE: April 1975
	6. PERFORMING ORGANIZATION CODE
7. AUTHOR(S): F. A. Record, R. M. Patterson, D. ... Bryant, and A. H. Castaline	8. PERFORMING ORGANIZATION REPORT NO. GCA-TR-75-11-G(1a)
9. PERFORMING ORGANIZATION NAME AND ADDRESS: GCA Corporation, GCA/Technology Division, Bedford, Massachusetts 01730	10. PROGRAM ELEMENT NO.
	11. CONTRACT/GRANT NO. 68-02-1376
12. SPONSORING AGENCY NAME AND ADDRESS: Environmental Protection Agency, Office of Air and Waste Management, Office of Air Quality Planning and Standards, Research Triangle Park, North Carolina 27711	13. TYPE OF REPORT AND PERIOD COVERED: Final
	14. SPONSORING AGENCY CODE
15. SUPPLEMENTARY NOTES	

16. ABSTRACT

This report presents a comparative discussion and evaluation of the modeling techniques available to assess the photochemical oxidant air quality impact of highway system modification or development. Five attributes of eight modeling techniques are discussed. The eight methods considered, in order of increasing complexity, are: (1) VMT Change, (2) Linear Rollback, (3) Nonlinear Rollback: Appendix J, (4) Gifford-Hanna Photochemical Model, (5) Statistical Relationships: Diffusion Kinetics Model, and (8) Urban Air Shed Photochemical Simulation Model. For each of these the following five attributes are discussed: (1) applicability and reliability, (2) data and manpower requirements, (3) use of the technique, (4) limitations, and (5) special features. The information presented in this report gives guidance towards choosing a model best suited to a given need, based on compatibility with these attributes.

17. KEY WORDS AND DOCUMENT ANALYSIS

a. DESCRIPTORS	b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Group
Highways Automotive Emissions Oxidant Oxidant Precursors Air Pollution Forecasting	Photochemical Oxidant Models Appendix J Relationships Linear & Non-linear Rollback Proportional Models	

18. DISTRIBUTION STATEMENT: Unlimited	19. SECURITY CLASS (This Report): Unclassified	21. NO. OF PAGES: 108
	20. SECURITY CLASS (This page): Unclassified	22. PRICE: 5.25

EPA Form 2220-1 (9-73)

ABSTRACT

This report presents a comparative discussion and evaluation of the modeling techniques available to assess the photochemical oxidant air quality impact of highway system modification or development. Five attributes of eight modeling techniques are discussed. The eight methods considered, in order of increasing complexity, are: (1) VMT Change, (2) Linear Rollback, (3) Nonlinear Rollback: Appendix J, (4) Gifford-Hanna Photochemical Model, (5) Statistical Relationships: Repro-Modeling, (6) Reactive Environmental Simulation Model, (7) Diffusion Kinetics Model, and (8) Urban Air Shed Photochemical Simulation Model. For each of these the following five attributes are discussed: (1) applicability and reliability, (2) data and manpower requirements, (3) use of the technique, (4) limitations, and (5) special features. The information presented in this report gives guidance towards choosing a model best suited to a given need, based on compatibility with these attributes.

CONTENTS

		Page
List of Figures		vi
List of Tables		vii
Sections		
I	Introduction and Summary	1
II	VMT Change	6
III	Linear Rollback	13
IV	Nonlinear Rollback: Appendix J	32
V	Gifford-Hanna Photochemical Model	45
VI	Statistical Relationships: Repro-Modeling	55
VII	Reactive Environmental Simulation Model	64
VIII	Diffusion Kinetics Model	77
IX	Urban Air Shed Photochemical Simulation Model	92

LIST OF FIGURES

No.		Page
1	Maximum 1-Hour Average Oxidant Concentrations as a Function of 6- to 9-a.m. Averages of total Hydrocarbon Concentrations at CAMP Stations, June Through September, 1966 Through 1968 and in Los Angeles, May Through October 1967	34
2	Maximum Daily 1-Hour Average Oxidants as a Function of 6- to 9-a.m. Averages of Nonmethane Hydrocarbons at CAMP Stations, June Through September, 1966 Through 1968, Los Angeles, May Through October 1967	35
3	Comparison of Curves for Total Hydrocarbons and Nonmethane Hydrocarbons With Appendix J	36
4	Comparison of Appendix J and Linear Rollback	37
5	Upper Limit of Maximum Daily Oxidant at Three Los Angeles County Stations, May Through October 1967	39
6	Comparison of Total Hydrocarbon Versus Oxidant Curve of AP-84 With Curve for Denver	41
7	Comparison of Nonmethane Hydrocarbons Versus Oxidant Curve of AP-84 With Curve for Los Angeles	42
8	Variation of Diffusitivity With Height for Different Stability Conditions	88

LIST OF TABLES

No.		Page
1	Summary Matrix of Photochemical Oxidant Modeling Techniques and Attributes	4
2	Data Requirements and Procedure Outline	18
3	Comparison of Observed Hourly Regional Average Concentrations of RH, NO_2, and O_3 With Concentrations Predicted by the Gifford-Hanna ATDL Model for Los Angeles, September 30, 1969	47
4	Comparison of Observed Hourly Average Concentrations of O_3, HC, and CO With Concentrations Predicted by the Gifford-Hanna ATDL Model at Five Locations in Denver, Colorado, August 13, 1973	48
5	Impact of Federal Emission Control Standards Mobile Sources – Oxidant (in pphm)	59
6	Effects of Single Day Traffic Reduction Policy on Air Quality (Oxidant, pphm)	60
7	Input Variable Constraints	62
8	Chemical Dynamics Module for REM	67
9	Estimated Maximum Time and Costs for Obtaining Traffic and Area Source Inputs for REM	72
10	Correlation Coefficients and Regression Equation for DIFKIN in Los Angeles	78
11	Percent Change in Predicted Concentrations of O_3, NO, NO_2, and HC for a 50 Percent Increase in Each of Various Model Parameters	80
12	Vehicular Emissions Data Required for DIFKIN	83
13	Stationary Source Emissions Data Required for DIFKIN	84
14	Photochemical Reactions and Rate Constants Used in DIFKIN	85

SECTION I

INTRODUCTION AND SUMMARY

This report presents a comparative discussion and evaluation of the available photochemical oxidant modeling techniques applicable to highway sysstm evaluation. The remainder of this report treats each of the eight techniques in separate sections, starting with the simplest and proceeding to the most complex.

The information presented in this report provides guidance towards choosing a model suitable to a given need. While not laying down strict guidelines, the report facilitates the choice of an appropriate model by discussing the following attributes of each modeling technique:

- Applicability and reliability
- Data and manpower requirements
- Application of the technique
- Limitations
- Special features

Once criteria are set for each of these attributes the choice of a model may become obvious. Alternatively, the discussion of these attributes presented in this report may help clarify the criteria to be met.

The following modeling techniques for assessing photochemical oxidant impact are evaluated in this report:

1. VMT Change
2. Linear Rollback

3. Nonlinear Rollback: Appendix J
4. Gifford-Hanna Photochemical Model
5. Statistical Relationships: Repro-modeling
6. Reactive Environmental Simulation Model
7. Diffusion Kinetics Model
8. Urban Air Shed Photochemical Simulation Model

The first three techniques are simple relationships between a surrogate for oxidant precursor concentrations and expected maximum oxidant concentrations. The third technique involves the Appendix J type curves and is the first to acknowledge the nonlinear relationship between precursor and oxidant concentrations. None of these techniques requires the use of a computer.

The Gifford-Hanna model is a transition from these simple models into the more complex ones. It may or may not require a computer depending on the characteristics of its use. It is the first technique in the list to include specific chemical reaction mechanisms.

Repro-modeling is a hybrid technique which develops statistical relationships between input parameters and calculated concentrations from another model. To date, a repro-model has been built only for Los Angeles based on the input and output of the Urban Air Shed Photochemical Simulation Model.

The last three models are all large computer codes. They treat atmospheric transport and diffusion processes, and atmospheric chemistry, with varying detail and computational complexity. Their predictive capabilities also vary, although this is verified only for Los Angeles. Techniques (6) and (7) are trajectory models which compute pollutant concentrations in a column of air being advected across a region. Thus, at any time, concentrations are estimated at only one (horizontal) spatial point and conversely. The last technique is a grid type model which calculates

concentrations at a number of points at any given time. These three techniques represent the state-of-the-art of photochemical oxidant modeling.

Table 1 presents a summary matrix of oxidant modeling techniques and the attributes listed above. The information presented in this table is discussed in the remainder of the report.

Table 1. SUMMARY MATRIX OF PHOTOCHEMICAL OXIDANT MODELING TECHNIQUES AND ATTRIBUTES

	Low → Complexity/cost → High							
	VMT change	Linear rollback	Nonlinear rollback	Gifford-Hanna	Statistical models	REM	DIFKIN	SAI model
Applicability	Screening procedure Small urban areas without oxidant problem	Screening procedure Small urban areas without oxidant problem	Screening procedure/ system level analysis	System level analysis	Repeated application Policy alternatives	Project or system level analysis	Project or system level analysis	System or project level analysis
Reliability	Good as a rough approximation	Good as a rough approximation	Good as a rough approximation. Better if location-specific curve is used.	Good for trends. Poor for concentrations.	Only as good as underlying model on which based.	Adequate for approximate concentration. Not well validated.	Good for approximate concentration. Better validated.	Good for approximate concentration. Not well validated.
Data requirements	Very low	Low	Low	Low to moderate as specified by user.	Low in use. High in development.	Fairly large emissions, meteorological and topographical input data requirement.	Large emissions and meteorological input data requirement.	Extensive emissions, meteorological, and topographical input data requirement.
Manpower to set up[a]	1-2 man-weeks	2-4 man-months	2-4 man-months	2-4 man-months	8 man-months to develop base. 2-3 man-weeks to build model.	4-6 man-months	6 man-months	8 man-months
Cost to run	--[b]	--[b]	--[b]	$280[c]	$10/case[d]	$50/trajectory[d]	$50/trajectory[d]	$1000/1-day[d] simulation

[a] These efforts are conservatively high and include collecting before and after VMT data, preparing emissions data, gathering air quality data, and putting all data in a form suitable for use.

[b] Insignificant

[c] Based on an average rate of $7.00 per manhour.

[d] Based on computer time (IBM 370/155) at an average cost of $15 per minute.

Table 1 (Continued). SUMMARY MATRIX OF PHOTOCHEMICAL OXIDANT MODELING TECHNIQUES AND ATTRIBUTES

	Low → Complexity/cost → High							
	VMT change	Linear rollback	Nonlinear rollback	Gifford-Hanna	Statistical models	REM	DIFKIN	SAI model
Limitations	Limited applicability	Limited applicability	Limited applicability. Results dependent on monitor locations.	Technically questionable	Reliability a function of basis model	Not well validated. Expensive.	Not well validated or documented. Expensive. Complex.	Not well validated. Expensive. Complex.
Features	Inexpensive screening procedure	Inexpensive screening procedure	Inexpensive screening procedure. Acknowledges reaction mechanisms.	Computer not necessary. Simple inclusion of reaction mechanisms and meteorology.	Inexpensive once developed. Allows repeated examination of various policy alterations.	Treats atmospheric transport and photochemical processes explicitly	Treats atmospheric transport, diffusion and photochemical processes explicitly	Treats atmospheric transport, diffusion, and photochemical processes explicitly. Develops concentration estimates over large area.

SECTION II

VMT CHANGE

APPLICABILITY AND RELIABILITY

Changes in concentration of photochemical oxidants and nitrogen dioxide have been defined by many simple functional relationships. The simplest relates changes in the pollutant levels with vehicle-miles of travel (VMT). The function assumes that changes in these variables, VMT, and pollutant concentrations, are linearly related. That is, for example, if VMT were to increase by 10 percent, concentrations would be assumed to increase by 10 percent.

By its very nature, the use of this approximation is considered to be limited. It is intended to be used as a substitute for extensive technical evaluations. It would be useful as an indicator of trends in air quality in areas not now experiencing violations of air quality standards for oxidants (the Priority III areas). Its purpose as a screening procedure allows for a rough estimation of the impact of a facility on the regional ambient air quality. If the results of the analysis indicate the possibility of a violation of the NAAQS, a more extensive analysis must be undertaken. This screening procedure, approximate in nature, is best restricted to areas where the growth in vehicular emissions is the greatest contributor to the growth in total emissions, because growth in stationary source emissions are not accounted for but could cause violations of air quality standards.

DATA AND MANPOWER REQUIREMENTS

Data requirements for the analysis of small changes in VMT due to facility construction are relatively minimal. Data needs are limited to air quality data and existing and projected vehicle-miles of travel (VMT).

The necessary air quality data would ordinarily be the second highest concentration of oxidants, and should be for a year as recent as possible. These air quality data would typically be available either from a regional air pollution control agency, state air agency, or EPA.

Vehicle miles of travel data are typically available from the ongoing transportation planning process. Sources of such data include the highway or planning agency. The technique utilized for determining VMT varies substantially among individual states. The most widely used and probably the most accurate method involves a highway link system from which VMT are calculated as a function of individual link length and average daily traffic (ADT) volume on the link. This technique appears to be used most widely in larger metropolitan areas where various regional transportation planning studies and highway inventories have been undertaken.

The second method involves estimating VMT based on motor fuel consumption. Generally, this is the method used for small urban and rural areas, and usually the data are presented in terms of statewide or regional VMT. While this particular technique is suitable for estimating gross VMT on a regional basis, it proves inadequate when knowledge of local VMT trends is required. Either technique appears satisfactory for the needs of this analysis, so long as the data are fairly current, are for the appropriate geographic area, and include all roads.

Manpower requirements are minimal since data are routinely collected by the planning agencies and can be recovered with minimum effort. To

identify, locate, and collect current VMT data, to adjust it to the year of interest, and to compare the project and no-project cases would be expected to require no more than 1 or 2 man-weeks over a calendar period of 2 to 4 weeks.

APPLICATION OF THE TECHNIQUE

This technique is based upon a simple linear relationship. The relationship can be expressed as a simple ratio:

$$\frac{VMT_e}{c_e} = \frac{VMT_p + VMT_e}{c_p + c_e} \qquad (1)$$

where VMT_e = existing VMT

VMT_p = projected increase to VMT due to facility

c_e = existing pollutant concentration

c_p = projected increase in concentration due to added VMT.

Because the purpose is to estimate the impact of a facility or of traffic growth on air quality to predict future concentrations, Equation (1) can be rewritten as follows:

$$c_f = c_p + c_e = \frac{c_e \left(VMT_p + VMT_e\right)}{VMT_e} \qquad (2)$$

where c_f = estimated projected pollutant concentration.

This relationship is utilized through the following steps:

1. Define the "baseline" year for the analysis. This must be the most recent year for which air quality data are available. Because of the time to collect, reduce, correct, and summarize air quality data, the baseline year being used may be 2 or 3 years prior to the current date. For example, transportation control plans now (in 1975) being prepared typically use 1972 or 1973 as the baseline year.

2. Define the geographic area. There is little scientific basis for selecting a geographic area for analysis when using such a crude technique. Too small an area (e.g., a minor civil division) would over-state the effect of traffic growth. The pragmatic approach is to use the geographic area also used as the base for the best VMT data avilable. Highway agencies typically report VMT for urbanized area, consisting of a central city and its surrounding densely settled districts, or for standard metropolitan statistical areas. Either of these may be adequate for defining the area of analysis, but neither will probably be representative of the AQCR in general. The use of a state-wide area should definitely be avoided, as the air quality will be insensitive to activity changes over such a large area.

3. Obtain the "present" VMT for the geographic area in question. Generally VMT data are available for every major urban area for some year within the past 2 or 3 years.

4. Adjust the VMT to be representative of the baseline year. This may require obtaining another year's set of VMT data or consulting with the highway agency to determine a basis for interpolation or extrapolation. Generally a linear fit will be perfectly satisfactory for this method.

5. Obtain the VMT for the project being evaluated. If the method is being used for areawide evaluation, obtain the VMT for the future year in question. If the project being evaluated will not be open until some future year, the VMT data may be for a future year. In such a case it will be necessary to perform one other step:

   a. Estimate the VMT from roads other than the project road for the future year, using extrapolation or interpolation. This provides a basis for determining the contribution to future VMT from the project alone, but is less accurate than (b) below because it relies upon the VMT air quality relationship remaining valid over time, which is doubtful, or

   b. Determine what VMT the project would involve if open in the baseline year. This requires estimating normal traffic growth, then subtracting the normal growth from the future year VMT estimate. This provides an estimate of the change in present air quality from the project under current conditions. In this case,

$$VMT_{pf} = VMT_{pp} (1 + G) \qquad (3)$$

where VMT_{pf} = future year VMT from proposed facility

VMT_{pp} = estimated present equivalent of VMT from proposed facility

G = normal growth in VMT in intervening years.

Typically, growth is a few percent per year. (the national average is about 5 percent per year.) The local growth rate should be obtained from the highway agency.

The project VMT to be used in Equation (3) is then:

$$VMT_{pp} = \frac{VMT_{pf}}{1 + G}.$$

6. Use Equation (3) to estimate the effect of tne project.

Because this is such a crude procedure, this technique should only be used for determining whether more sophisticated tools are needed. If the method predicts that air quality standards may be violated, resources should be allocated for better air quality data, analysis, and projections, perhaps using one of the methods discussed in later sections of this manual.

LIMITATIONS

This technique is applicable as only a rough screening procedure under limited conditions. Its validity is restricted to areas where vehicular emissions are the major source of growth in ambient concentrations of oxidants. This procedure yields an estimation of the impact on air quality due to changes in VMT. If results indicate the possibility of a violation in the NAAQS, extended analyses of the types to be discussed in later sections of this work would be required.

A major limitation of this model is that it neglects the pollution control effects of the Federal Motor Vehicle Emissions Control Program and thus tends to over-predict future contributions of vehicular sources to total emissions and ambient concentrations. This may, however, tend to compensate for the lack of consideration of nonvehicular sources.

Two other major factors of pollutant concentrations are ignored, vehicular speeds and stationary sources. Vehicular emission rates vary with speed. Hydrocarbon emissions decrease with speed while NO_2 emissions have been shown to increase at higher speeds. Uncertainty occurs when speeds are not explicitly treated. Generally speaking, however, sources which would generate significant additional VMT necessitating an air quality review would typically be high capacity limited access highway facilities. Speeds would tend to be greater than existing average network speeds. Measured concentrations should theoretically be a function of speed (the next section deals with this concept) thus introducing the possibility for error in the prediction of pollutant concentrations. This error would be an over-estimate for hydrocarbon emissions and an under-estimate for nitrogen dioxide emissions.

Stationary sources may contribute greatly to regional pollutant concentrations. The contributions would vary depending upon local characteristics such as density and amount of industrialization. Without a proper stationary source emission inventory, these sources cannot be treated explicitly. Since the procedure is intended to be "quick and dirty," exogenous consideration is all that is required. As with the treatment of speeds, uncertainties introduce errors that would appear as over-estimates.

SPECIAL FEATURES

This technique, although based on gross assumptions, is a reasonable screening procedure for areas that are not now in violation of the ambient standards or that do not have expertise or funds for air quality

forecasting. The data are easily obtainable with minimum manpower requirements. Thus the procedure is applicable to many smaller urban areas where sophisticated data collection procedures have yet to be implemented. Use of the technique lends itself to restricted budgets, since the simple linear expression does not involve computer modeling or difficult computational processing.

SECTION III

LINEAR ROLLBACK

APPLICABILITY AND RELIABILITY

This technique employs the same relationships as the previous one, except that oxidant precursor emissions are substituted for VMT. This technique is somewhat more reliable than the technique discussed in Section II due primarily to three basic refinements: (1) the inclusion of speed data, (2) accounting for the Federal Motor Vehicle Emission Control Program, and (3) accounting for stationary source emissions. Like the first technique, this technique is a reasonable screening procedure under limited conditions. Its use would be applicable to areas where sophisticated techniques cannot be used, preferably areas not yet in violation of ambient air quality standards.

This procedure can be used to produce results exhibiting the emissions contribution of a proposed facility, or it can be used for assessing general growth. The simple relationship of the previous technique is extended by treating an additional function of vehicular emission rate, that being speed, and also accounting for the Federal Motor Vehicle Emissions Control Program (FMVECP). The speed data are required in order to compute actual emissions instead of working strictly with VMT as with the previous technique. The inclusions of speed permits the use of emission factors adjusted for variations in speed from such sources as AP-42.[1] A greater degree of accuracy can be expected since speed is no longer implicitly fixed in the relationship but rather behaves as a controlling parameter.

Additional accuracy is obtained by the explicit treatment of stationary source emissions. These sources may contribute significantly to the total emissions, but are unaffected by changes in the transportation network. Therefore, by accounting for their contributions, results are obtained which allow for more accurately predicting the role of transportation projects (or general growth) in total emissions increases. This therefore allows assessment of the contribution of transportation to areawide pollutant burden, and provides an indicator of the future air quality.

DATA AND MANPOWER REQUIREMENTS

The problem of estimating emissions from motor vehicles is basically one of specifying a number of parameters, and then multiplying these parameters together with suitable emission factors to compute roadway emission strengths. Differences among methods of estimating emissions arise in the nature and comprehension of the input parameters. The basic algorithm is essentially the same for all the methods. The adjustment factors vary depending on specific requirements and data availability.

The basic data requirements for a highway-related emission model consist of the following: emission factors, base and projected vehicle miles of travel (VMT), and speed. As for the previous technique, these data would usually be available from the local, regional or state transportation planning agencies. In the case that the data are unavailable from these sources, except for VMT, the data could reasonably be developed from current literature* at the expense of additional manpower.

---

*National average statistics could be substituted or acceptable data could be developed from such sources as the Highway Capacity Manual. Some models, such as the Special Area Analysis (SAPOLLUT), include default values as substitutes for unavailable data.

Additional variables could be introduced so that the approach would be responsive to local conditions. Typical parameters would include the mix of vehicles, type and location of highway, and degree of congestion.

The data could be aggregated according to total vehicle-miles of travel by class of vehicle on various roadways by roadway functional classification. EPA vehicular classification standards, 40 CFR part 85, used to determine total emissions, are composed of the following categories:

1. Light-duty gasoline vehicles (automobiles).
2. Light-duty gasoline trucks.
3. Light-duty diesel vehicles.
4. Heavy-duty gasoline vehicles.
5. Heavy-duty diesel vehicles.
6. Motorcycles.

The above listing attempts to identify categories of vehicles that generally tend to exhibit common characteristics with regard to pollutants emitted per mile of travel. The distribution of vehicle types can be established through vehicle classification inventories supplemented by vehicle registration data obtained from state agencies or private concerns such as the R. L. Polk Company.

Since the volume of nitrogen dioxide and hydrocarbons produced per vehicle-mile is related to vehicular speed and since average speed varies with the roadway classification, it may be important that the distribution of total VMT by roadway classification be identified. (Grouping roads by speed or functional classification reduces the computational effort compared to calculating emissions separately for each road.)

Typically roadway classifications are categorized as: (1) freeways/expressways; (2) arterials; (3) collector/distributors; and (4) local streets. These general classifications are associated with different characteristics of speed and operating efficiency.

The criteria for determining the functional classification of a street system has been well established and documented by the Institute of Traffic Engineers, the Transportation (Highway) Research Board, and others.

Speed data could be averaged throughout the day or disaggregated into either an hourly distribution or periods of the day. The value of either of the disaggregated approaches is the introduction of the effects of congestion on speeds and therefore emissions. The SAPOLLUT Program[2] for air quality analyses, for instance, has been developed with endogenous default values for hourly distributions of ADT for utilization if local data are unavailable. Based on the Highway Capacity Manual and the findings of other studies, volume capacity ratios are computed to generalize a relationship to speed. The explicit treatment of speed and other parameters by SAPOLLUT extends the validity of its results.

Manpower requirements are considerably greater than for the VMT analyses of Section II. Significant additional data collection, reduction and processing is required to prepare input for the modeling process. Much of the data are part of the normal 3-C planning process efforts; however, some data, not part of the routine output, can be obtained through development of appropriate summary programs or clerical efforts. The 3-C process can be expected to provide access to most of the typical regional transportation and land use statistics. In most cases where specific elements of data are not readily available or recoverable, default values such as those included in the SAPOLLUT program are acceptable for use in the computation of emissions or emission changes since the intention of this technique, as with the previous technique, is that of a reasonable screening procedure.

An additional requirement would be to have or to prepare a stationary source emission inventory. These sources may significantly contribute to total regional emissions. Stationary sources are unaffected by changes in the transportation network. Thus, concerned with the impact of additional highway network capacity upon air quality, contributions of the stationary sources should be factored out of the total existing measurements. This inventory should be available for most urban areas. In the case where it is not available and budgets for local environmental analyses are constrained, another technique should be chosen. But if the time and money could be obtained or are available, the completion of a stationary source inventory would be recommended.

Data requirements and the procedure outline are tabulated in Table 1. The collection and adjustment for the VMT data is discussed in Section II. Speed information is usually available from the planning model used by the local planning agency, but it is only approximately equivalent to true speeds. The stationary source inventory explicitly accounts for nonvehicular emissions. The specific data required by a particular emissions model, as previously discussed, explicitly accounts for local conditions which affect local vehicular emissions characteristics (vehicle age distribution, etc.).

Basic design variables for the highway of concern will provide for the classification of the roadway type, and the projected VMT, which can be adjusted either for the base year or for a desired analysis year as discussed with regards to the previous technique. Emission adjustment factors will account for variations in speed, vehicle mix, and the vehicle age distribution.

The total effort for the data collection and processing stages and the required computations for analysis and evaluation is estimated to require at least 1 man month. Typically the total requirement would range from the minimum of 1 month to 3 or 4 man months. In some cases these estimates could conceivably be considerably low. In all cases the use of

Table 2. DATA REQUIREMENTS AND PROCEDURE OUTLINE

Data	Task
EXISTING - DATA COLLECTION	
VMT	Collect and adjust to base year
Air Quality Data	Second highest reading for base year
Speed	VMT-weighted daily average speed by roadway classification, or nearest approximation.
Stationary Source Inventory	Determine contribution to total emissions (reactive HC only)
Model-specific	Special data requirements of selected emissions model
FUTURE - DATA COLLECTION	
Highway facility	Obtain design variables for analysis
VMT	Projection for analysis year or base year for facility of concern.
Emission adjustment factors	Obtain information needed for determining emission factors, such as speed, vehicle mix and age distributions.
ANALYSIS COMPUTATIONS	
Final preparation	Prepare data for selected model's input requirements.
Model run	Computer computations, Analysis and Evaluations.

computer facilities could, to varying degrees, be substituted for manual computations and processing to reduce the total calendar months required for the project.

APPLICATION OF THE TECHNIQUE

Emission Computations

There are numerous methods for estimating emissions from motor vehicles.[1-8] The basic algorithm is essentially the same for the various methods. By the method given in EPA publication AP-42[1], emission strengths for exhaust hydrocarbons and oxides of nitrogen are calculated by:

$$e_{np} = \sum_{i = n - 12}^{n + 1} C_{ip} \, d_{ipn} \, m_{in} \, S_{ip} \qquad (4)$$

where e_{np} = emissions (grams per vehicle mile) for calendar year n and pollutant p,

c_{ip} = emissions (grams per vehicle mile) for pollutant p for i^{th} model year at low mileage at an average speed of 19.6 miles per hour.

d_{ipn} = emission deterioration factor for the i^{th} model year, calendar year n, and pollutant p for vehicles with emission controls,

m_{in} = weighted annual travel of the i^{th} model year during calendar year n,

and S_{ip} = weighted speed adjustment factor for exhaust emissions of pollutant p for the i^{th} model year.

The weighted speed correction factor, S_{ip}, is in turn computed by the relation:

$$S_{i_m p} = \sum_{j=1}^{k} f_{j_m} v_{jp} \qquad (5)$$

with $S_{i_m p}$ = weighted speed adjustment factor for exhaust emissions of pollutant p for the i^{th} model year during calendar year m,

f_{j_m} = the fraction of the total annual vehicle miles traveled at speed j during calendar year m,

v_{jp} = the average speed correction factor for average speed j and pollutant p,

and k = total number of different average speeds.

Curves of v_{jp} versus speed are shown on Figure 3.1.1-1 of AP-42. Values of the other parameters will be discussed later with other methods.

Evaporative and crankcase hydrocarbon emissions are calculated by:

$$f_n = \sum_{i=n-12}^{n+1} h_i m_{in} \qquad (6)$$

where f_n = combined evaporative and crankcase hydrocarbon emissions for calendar year n,

h_i = combined evaporative and crankcase emission rate (grams per vehicle mile) for the i^{th} model year,

and m_{in} was defined previously.

To calculate actual emissions, e_{np} and f_n must be multiplied by the number of vehicle miles traveled (VMT) for the region of interest during a given time period.

As mentioned earlier, the real differences among vehicle emission models do not arise from the computational methods, but rather from the extent and definition of the input parameters. It can be stated that, in general, newer methods will provide better results because of improved input data,

and perhaps because experience provides for improved specification of input parameters.

Additional methods[2,3,4,5] have been given for computing motor vehicle emissions; almost all use the same basic technique described for AP-42 and all require the same basic data.

A recent technique[6] distinguishes between "hot starts" and "cold starts" in calculating emissions. Cold start data are obtained from the Federal Test data (AP-42) by assuming a fraction of the test results of total emissions to have occurred during the first 2 minutes or cold start portion of the cycle. This fraction varies with year and is based on General Motors tests results. The grams per mile emissions during the "hot" portion of the test are calculated from the remaining portion of the test sample. The hot emissions are subtracted from the cold emissions to determine the excess emissions attributable exclusively to cold start. The result is a new set of emissions data (grams per mile) for use with VMT data, and a set of "cold start" emissions to be applied where these conditions obtain.

The method has been carried further[7] to define a range of "fractions of a cold start" which increase with an increase in soak time. Starts after a 12-hour soak are considered to be fully cold.

EPA has recently published a supplement[8] revising the internal combustion engine sources portion of AP-42. The new methodology for estimating emissions is quite different from that previously employed and described above due mainly to three factors:

- The new method does not include deterioration factors
- "Cold start" and "hot start" emissions are included
- Emissions projections are given in an appendix and not listed in the main section dealing with internal combustion engine sources.

The emission factors which are presented in this supplement are based on measurements taken during EPA's annual surveillance programs and cover calendar years 1971 and 1972. Deterioration is accounted for implicity in the emission factors for the year of measurement. For example, emission factors are presented as X grams per kilometer of exhaust hydrocarbons for a 1969 model year vehicle in calendar year 1972.

Other changes in the method of estimating motor vehicle emissions can best be described by examining the new algorithms used to compute emissions. For light-duty vehicles (automobiles) and light-duty trucks this is:

$$e_{npstw} = \sum_{i=n-12}^{n} c_{ipn}\, m_{in}\, v_{ips}\, z_{ipt}\, r_{iptw} \qquad (7)$$

where e_{npstw} = Composite emission factor in g/km (g/mi) for calendar year n, pollutant p, average speed s, ambient temperature t, and percent cold operation w.

c_{ipn} = The FTP (1975 Federal Test Procedure) mean emission factor for the i^{th} model year light-duty vehicles during calendar year n and for pollutant p,

m_{in} = The fraction of annual travel by the i^{th} model year light-duty vehicles during calendar year n,

v_{ips} = The speed correction factor for the i^{th} model year light-duty vehicles for pollutant p and average speed s,

z_{ipt} = The temperature correction factor for the i^{th} model year light-duty vehicles for pollutant p and ambient temperature t,

r_{iptw} = The hot/cold vehicle operation correction factor for the i^{th} model year light-duty vehicles for pollutant p, ambient temperature t, and percent cold operation w.

The discussion of these variables applies to automobiles and light trucks except where noted.

FTP Emission Factor (c_{ipn}) - These data are divided by geographic area into : low altitude (non-California), high altitude, and California only. The tabulated values are applicable to calendar years 1971 and 1972 (only 1972 for trucks). California emission factors are presented separately since California vehicles have been, in the case of several model years, subject to emission standards which differ from those standards applicable to vehicles under the Federal emission control program. For those model year California vehicles which did not have separate emission standards, the national emission factors are assumed to apply in California as well. Emissions at high altitude are differentiated from those at low altitude to account for the effect that altitude has on air-fuel ratios and concomitant emissions. The tabulated values are applicable to calendar years 1971 and 1972 (only 1972 for trucks) for each model year.

Fraction of Annual Travel by Model Year (m_i) - No significant change has occurred from previous emission estimation methods.

Speed Correction Factors (v_{ips}) - Speed correction factors enable the "adjustment" of FTP emission factors to account for differences in average route speed. Since the implicit average route speed of the FTP is 19.6 miles per hour (31.6 kph), estimates of emissions at higher or lower average speeds require this correction.

It is important to note the difference between "average route speed" and "steady speed." Average route speed is trip-related. It is based on a composite of the driving modes (idle, cruise, acceleration, deceleration) encountered in, for example a typical home-to-work trip. Steady speed is highway facility-oriented. For instance a group of vehicles traveling over an uncongested freeway link (volume/capacity

of, say, 0.1) might be traveling at a steady speed of about 55 mph (89 kph). Note, however, that steady speeds, even at the link level, are unlikely to occur where resistance to flow occurs (unsynchronized traffic signaling, congested flow, etc.).

Previously, the limited data available for correcting for average speed were presented graphically. Recent research has resulted in revised speed relationships by model year. To facilitate the presentation, the data are given as equations of the form:

$$v_{ips} = \exp (A + BS + CS^2) \qquad (8)$$

where S is the speed in miles per hour.

The values of the coefficients A, B, and C apply only for the range of the data, from 24 to 72 kilometers per hour (15 to 45 miles per hour). Since there is a need, in some situations, to estimate emissions at very low average speeds, correction factors have been developed for this purpose for 8 and 16 kph (5 and 10 mph).

Temperature Correction Factor (z_{ipt})

The 1975 FTP requires that emissions measurements to be made within the limits of a relatively narrow temperature band (68° to 86° F). Such a band facilitates uniform testing in laboratories without requiring extreme ranges of temperature control. Present emission factors for motor vehicles are based on data from the standard Federal test (assumed to be at 75° F). The correction factors are expressed in equational form and can be applied between 20°F and 80°F. For temperatures outside this range, the appropriate endpoint correction factor is applied.

Hot/Cold Vehicle Operation Correction Factor (r_{iptw})

The 1975 FTP measures emissions over three types of driving: a cold transient phase (representative of vehicle start-up after a long engine off period), a hot transient phase (representative of vehicle start-up after a short engine-off period), and a stabilized phase (representative of warmed-up vehicle operation). The weighting factors used in the 1975 FTP are 20 percent, 27 percent, and 53 percent of total miles (time) in each of the three phases respectively. Thus, when the 1975 FTP emission factors are applied to a given region for the purpose of assessing air quality, this can be viewed as if 20 percent of the light-duty vehicles in the area of interest are operating in a cold condition, 27 percent are operating a hot start-up condition, and 53 percent are operating in a hot stabilized condition. For non-catalyst vehicles (all pre 1975 model year vehicles), emissions in the two hot phases are essentially equivalent on a grams/kilometer (grams/mile) basis. Therefore, the 1975 FTP emission factor represents 20 percent cold operation and 80 percent hot operation.

There are many situations where these particular weighting factors may be inappropriate. For example, light-duty vehicle operation in the center city may have a much higher percentage of cold operation during the afternoon peak when work-to-home trips are at a maximum and vehicles have been soaking for 8 hours. The hot/cold vehicle operation factor allows the cold operation phase to range from 0 percent to 100 percent of total light-duty vehicle operations. This correction factor is a function of the percent of cold operation, w, and the ambient temperature, t. The correction factor is:

$$r_{iptw} = \frac{w + (100-w)f(t)}{20 + 80f(t)} \qquad (9)$$

where f(t) is a function of temperature presented in AP-42, Supplement No. 5.

The new methodology also allows for calculating evaporative emissions of hydrocarbons and idle emissions of hydrocarbons, nitrogen oxides, and carbon monoxide.

Emissions from light-duty, diesel-powered vehicles are calculated as before, except that the emission factors are given for pre-1973 model years. Projection to future years is given as an appendix.

Emissions from heavy-duty gasoline vehicles are calculated by:

$$e_{nps} \sum_{i=n-12}^{n} c_{ipn} m_{in} v_{ips} \qquad (10)$$

where the factors were defined previously. For heavy-duty diesel-powered vehicles the model year distribution is omitted:

$$e_{nps} = \sum_{i-n-12}^{n} c_{ipn} v_{ips}. \qquad (11)$$

Values for c_{ipn} are based on tests of vehicles on-the-road over the San Antonio Road Route (SARR). The SARR, located in San Antonio, Texas, is 7.24 miles long and includes freeway, arterial and local/collector highway segments. Since the SARR is an actual road route, the average speed varies depending on traffic conditions at the time of the test. However, the average speed tends to be around 29 kph (18 mph) with about 20 percent of the time spend at idle. The test procedure emission factor is composed entirely of warmed-up vehicle operation. Based on a preliminary analysis of vehicle operation data, HDV operation is primarily (about 95 percent) warmed-up.

Of course, it is quite necessary to estimate motor vehicle emissions beyond calendar year 1972, and this capability is provided in an

appendix to the revised AP-42. This is done purposely to separate the analytical results of EPA's surveillance testing program from what are acknowledged to be "best guesses" of future emission factors. There are several reasons for this separation. First, current legislation allows for limited time extensions for achieving the statutory motor vehicle emission standards. Secondly, Congressional action changing the time table for achieving these standards and/or changing their levels is likely in the future. Thirdly, new data on catalyst-equipped (1975 automobiles) are becoming available. The methods presented in the appendix for estimating emissions are similar to those described above.

There is a final source of data which might prove useful, especially for estimating emissions from higher speed, highway traffic. This is the Modal Analysis Model[9] developed for EPA. This model predicts emissions from a single vehicle or an ensemble of vehicles for a user-specified age distribution over any desired driving sequence within the range of the applicability of the model. The key point for highway traffic is that the model can predict emissions which reflect a constant cruise speed, not an "average route speed" which might include stops and starts. With proper resources, the model could even be used to estimate average emissions for a given urban area based on the typical driving cycle for that area instead of on the Federal Test Procedure.

Estimating Pollutant Concentrations by Linear Rollback

The linear rollback technique provides a means for converting total emissions to pollutant concentrations. The technique assumes that the concentration of a pollutant is equal to the background concentration of that pollutant plus some linear function of the emission rate of the pollutant, or:

$$c_t = c_b + k\,e \qquad (12)$$

where c_t is the total concentration of the pollutant

c_b is the background concentration of the pollutant resulting from natural sources

e is the total emissions of the pollutant for a particular averaging period, typically 24 hours

k is a constant

Generally c_b is a very small fraction of c_t and is often neglected. The total emissions, e, can be calculated or derived from inventories of emissions. Therefore, in an area where the concentration of a pollutant is monitored, the only unknown is the value of k. Because all other elements of the equation are known, it is a simple matter to calculate k. The equation in its most common form is expressed as $e/c = k$. The value of k is often referred to as the e/c ratio.

In determining the reduction in emissions required in a particular area in order to meet National Ambient Air Quality Standards (NAAQS), the second highest validated concentration is usually used with the contemporary emissions to determine the corresponding k value. The allowable emissions are then determined as follows:

$$e_a = c_s\,k \qquad (13)$$

where e_a is the estimated allowable or "safe" emission rate

c_s is the National Air Quality Standard for the pollutant (for ozone, $c_s = 0.08$ ppm)

k is a constant

The emissions reduction required, then, is equal to the difference between the baseline emissions and the calculated allowable emissions or, expressed as a percent reduction:

$$\% \text{ reduction required} = \frac{(\text{baseline emissions})-(\text{allowable emissions})}{\text{baseline emissions}} \times 100 \quad (14)$$

The chief advantages of the rollback model are that it is relatively simple and straightforward to use, and its theoretical basis is readily understood. While the technique does have various limitations, these are judged to be not so severe as to preclude its use in air quality analyses. The most important limitations of the model include its insensitivity both to spatial resolution with regard to the source-receptor relationship, and to local variations in meteorology and topography that occur within a region.

LIMITATIONS

This technique is applicable as only a screening procedure under limited conditions. The purpose of these models is as an analysis technique to determine the impact upon regional emissions due to an addition to the highway network or to estimating regional growth effects. Results could be interpreted to determine the possibility of violations to the NAAQS, through the linear rollback approach (as presented). The performance of air quality modeling efforts, to be discussed in the next sections, would be indicated if the occurrence of a violation in standards is forecasted with the method described here.

This technique introduces parameters which improve its reliability as compared with that of Section II. However, the forecasted pollutant concentration remains a linear function of the emission rate. This limitation is judged to be not so severe as to preclude utilization for the limited condition previously mentioned.

SPECIAL FEATURES

These emission computation techniques, relative to Technique 1, are significantly more reliable. The models are constructed to consider variables of speed and stationary source emission endogenously. The FMVECP is explicitly accounted for through the use of available emission factors. Data needed are available from typical regional planning data collection efforts. These emissions models are easily utilized and may be suitable for smaller areas or those not yet exhibiting violations of oxidants standards. Also, the data requirements of these models are consistent with smaller urban areas where data collection efforts may not be as sophisticated as those for large metropolitan regions.

REFERENCES

1. Compilation of Air Pollutant Emission Factors. EPA Report AP-42 (Second Edition). April 1973.

2. Special Area Analysis. (SAPOLLUT Model), U.S. DOT, August 1973.

3. Kircher, David S. and Donald P. Armstrong. An Interim Report on Motor Vehicle Emission Estimation. EPA-450/2-73-003, October 1973.

4. Wolsko, T. D., M. T. Matthies, and R. E. Wendell. Transportation Air Pollution Emissions Handbook. Argonne National Laboratory Report ANL/ES-15. July 1972.

5. Sauter, G. C. and W. R. Ott. A Computer Program for Projections of Vehicular Pollutant Emissions in Urban Areas, JAPCA, 24:54. No. 1. January 1974.

6. Wendell, R. E., J. E. Norco, and K. G. Groke. Emission Prediction and Control Strategy: Evaluation of Pollution from Transportation Systems, JAPCA, 23:91. No. 2. February 1973.

7. Cirillo, R. R., J. E. Norco, and T. D. Wolsko. The Effect of Cold Start on Motor Vehicle Emissions and Resultant Air Quality. Paper 74-127, 67th Annual Meeting, Air Pollution Control Association. Denver. 1974.

8. Supplement No. 5 for Compilation of Air Pollutant Emission Factors EPA Report AP-42 (Second Edition). Unedited copy. April 1975.

9. Automobile Exhaust Emission Modal Analysis Model, EPA Report EPA-460/3-74-005. January 1974.

SECTION IV

NONLINEAR ROLLBACK: APPENDIX J

Linear and nonlinear rollback are based on the assumptions that changes in concentrations are either directly or indirectly proportional to changes in total emissions and that such relationships can be defined. The assumption that changes in ambient concentration levels are proportional to changes in total emissions, as described in Section III for linear rollback, is reasonable if the existing spatial and temporal distributions of emissions remain constant.[1]

The effects of meteorology on ambient concentrations are included implicitly by the dependence on ambient concentrations. For long time periods or for worst case values, this lack of explicit dependence on meteorology is not critical.

APPLICABILITY AND RELIABILITY

For highway evaluation on both the project and system level, the requirement for unchanging emissions distributions in time and space is not met, since both project and system level modifications will likely lead to VMT changes. An additional problem with the application of linear rollback to photochemical oxidants is that oxidant concentrations depend, in a nonlinear fashion, on ambient concentrations of hydrocarbons and oxides of nitrogen. Nonlinear or modified rollback attempts to account for this nonlinearity through an empirically derived relationship between

maximum daily 1-hour average oxidant concentrations and 6 to 9 a.m. average concentrations of hydrocarbons. Hydrocarbon concentrations are then assumed to depend linearly on emissions, so that a relationship between changes in hydrocarbon emissions and oxidant concentrations is achieved. One form of this relationship is the Appendix J curve of the EPA regulations on preparation of implementation plans (40CFR51).

Figure 1 shows observed relationships[2] between maximum daily 1-hour oxidant concentrations and 6 to 9 a.m. average concentrations of total hydrocarbons. The approximate upper-limit observed oxidant curve forms an "envelope" around the maximum oxidant concentrations.

Figure 2 shows similar relationships of oxidant with nonmethane hydrocarbons;[2] that is, those considered to be reactive in photochemical oxidant formation. Again, the approximate upper-limit observed oxidant curve forms an envelope around the maximum oxidant concentrations.

Both of the envelope curves from Figures 1 and 2 are plotted on Figure 3, converted to yield the percentage reduction in hydrocarbon emissions (total and nonmethane) required to meet the oxidant standard. The Appendix J curve is also plotted on Figure 3, and it falls between the total hydrocarbon (lower) and nonmethane hydrocarbon (upper) curves.

Both the linear and nonlinear rollback models have been used in Transportation Control Plan development and evaluation. Figure 4 is a comparison of the nonlinear rollback of Appendix J with the results of assuming linear rollback, or a linear relationship between hydrocarbons and oxidants. The method has been to determine what hydrocarbon emission levels are consistent with meeting or maintaining the NAAQS for oxidant, although NO_x concentrations are also important. An additional problem with the use of proportional models for oxidant is that a period of time is required for the reactions which form oxidant to proceed. The air at

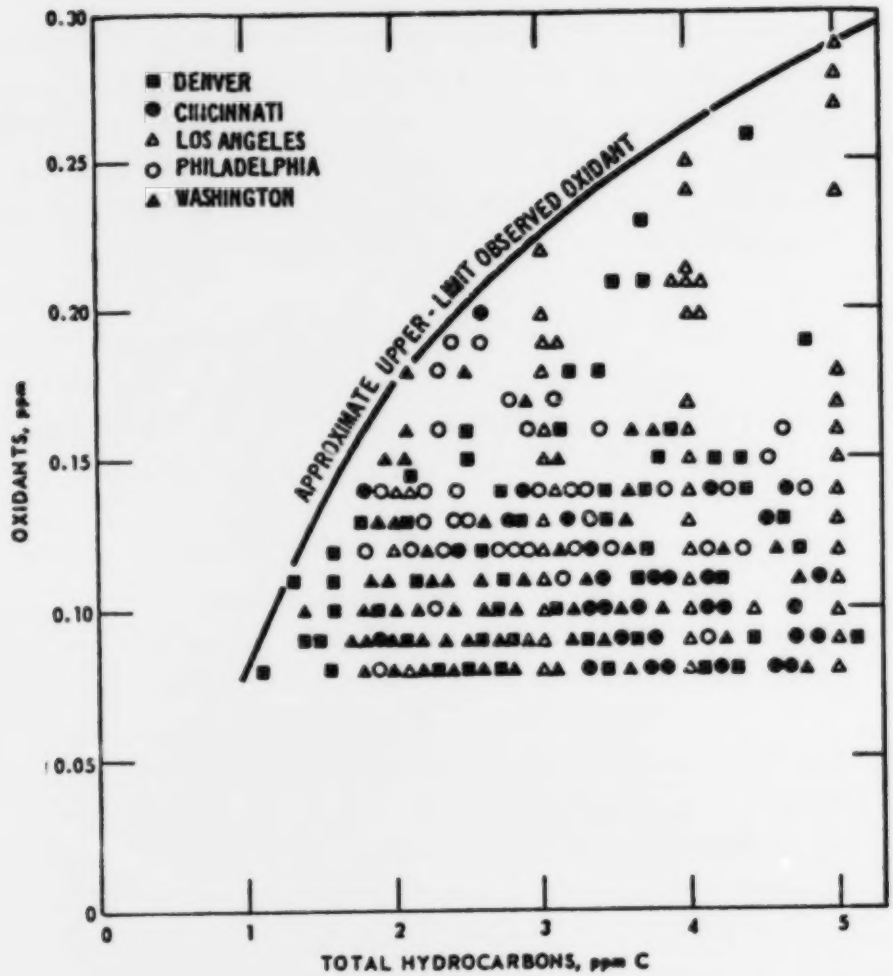

Figure 1. Maximum daily 1-hour average oxidant concentrations as a function of 6- to 9-a.m. averages of total hydrocarbon concentrations at CAMP stations, June through September, 1966 through 1968 and in Los Angeles, May through October 1967[2]

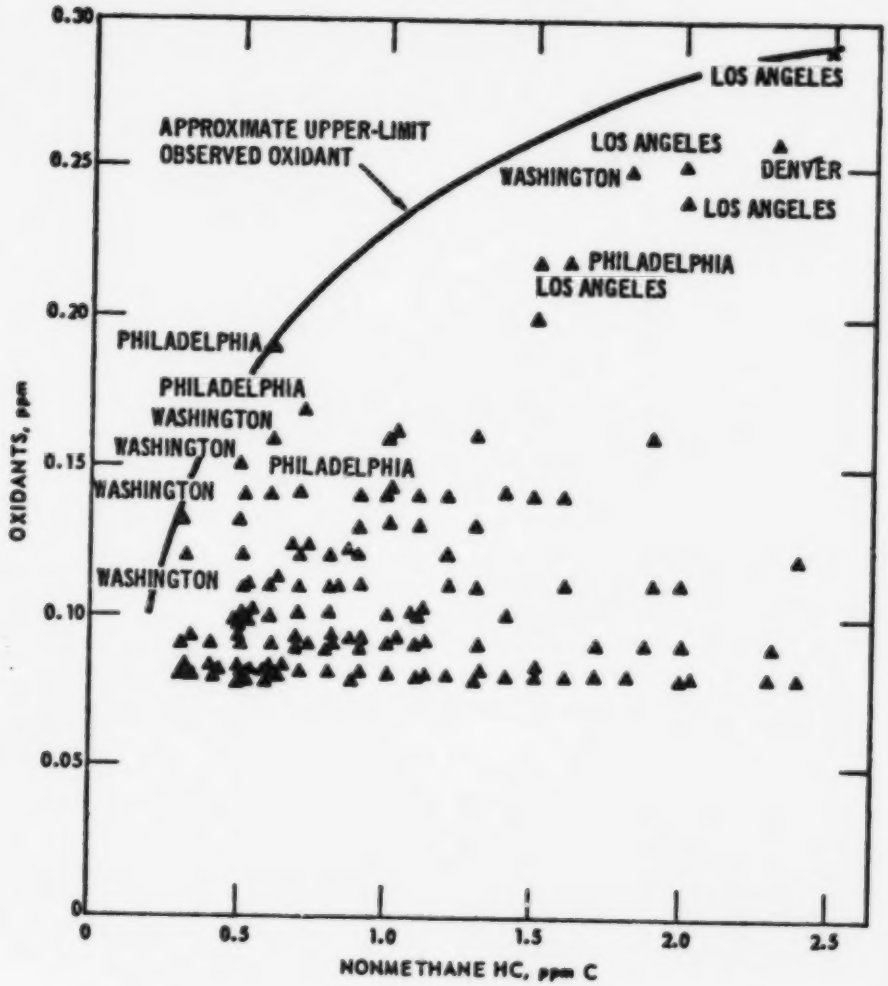

Figure 2. Maximum daily 1-hour average oxidants as a function of 6- to 9-a.m. averages of nonmethane hydrocarbons at CAMP stations, June through September, 1966 through 1968, Los Angeles, May through October 1967[2]

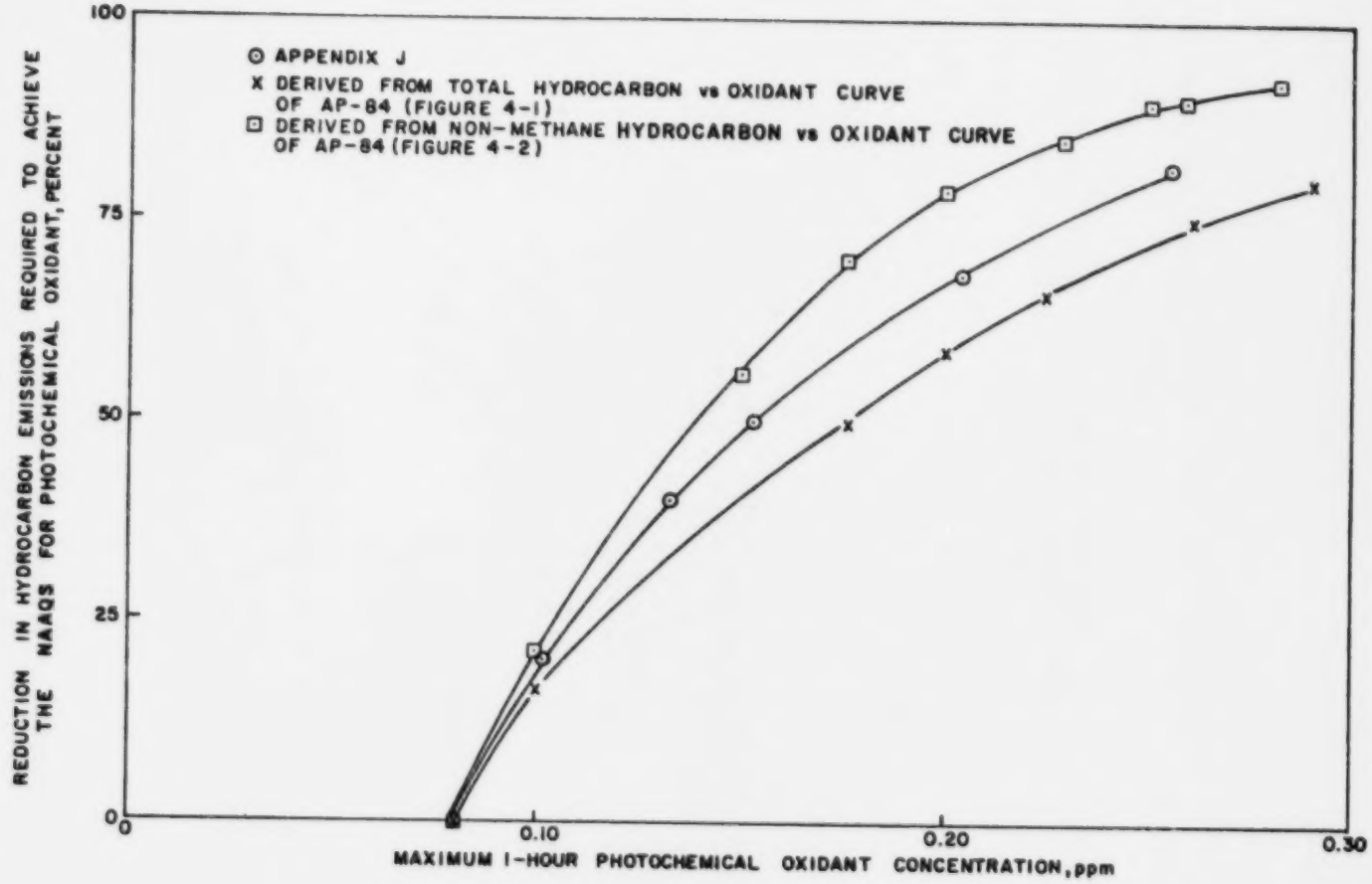

Figure 3. Comparison of curves for total hydrocarbons and nonmethane hydrocarbons with Appendix J

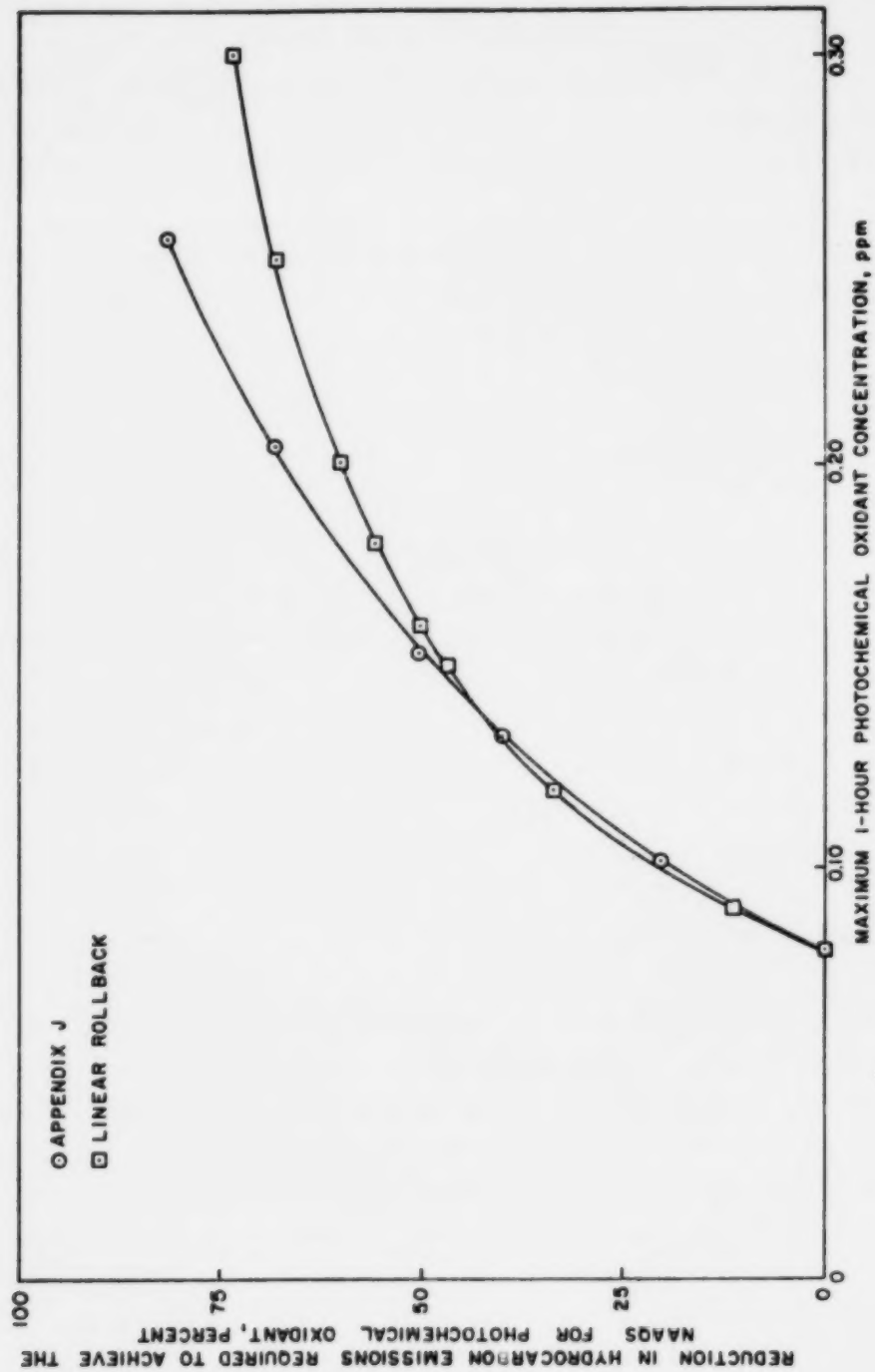

Figure 4. Comparison of Appendix J and linear rollback

a monitoring location in the morning 6 to 9 a.m. period is different from the air at that location during the afternoon oxidant peak. The two concentrations cannot strictly be related. This effect is shown in Figure IV-5.[3] The predominant summer wind in Los Angeles is southwesterly; that is, from downtown Los Angeles towards the USC Medical Center (3 miles away) and Pasadena (13 miles away). This figure suggests that higher concentrations of oxidant are experienced downwind after the photochemical reactions have had time to proceed. It also suggests that this effect becomes smaller as the mixing of pollutants improves, as evidenced by the closing of the curves at lower hydrocarbon concentrations.

DATA AND MANPOWER REQUIREMENTS

Nonlinear rollback models require only slightly more effort to apply than the previous technique in Section III. This would arise if location-specific curves are prepared as described later in this section. This should require no more than about 1 manweek. To use these curves to assess the oxidant impact from highways, the only data requirements are the second highest hourly average oxidant concentration and the percentage change in hydrocarbon emissions brought about by the proposed highway or system change.

APPLICATION OF THE TECHNIQUE

Methods for determining hydrocarbon emissions have been described in Section III. To apply a proportional model, only the peak (or second highest) 1-hour average oxidant concentration needs to be known. Using a linear model, the expected peak oxidant levels would be determined by a simple ratioing technique. The present peak oxidant value is multiplied by the ratio of projected to present hydrocarbon emissions to estimate the expected peak oxidant concentration. In doing this, one must decide upon the size of the area to be used for the analysis. No real guidance is available to assist in this determination, and this

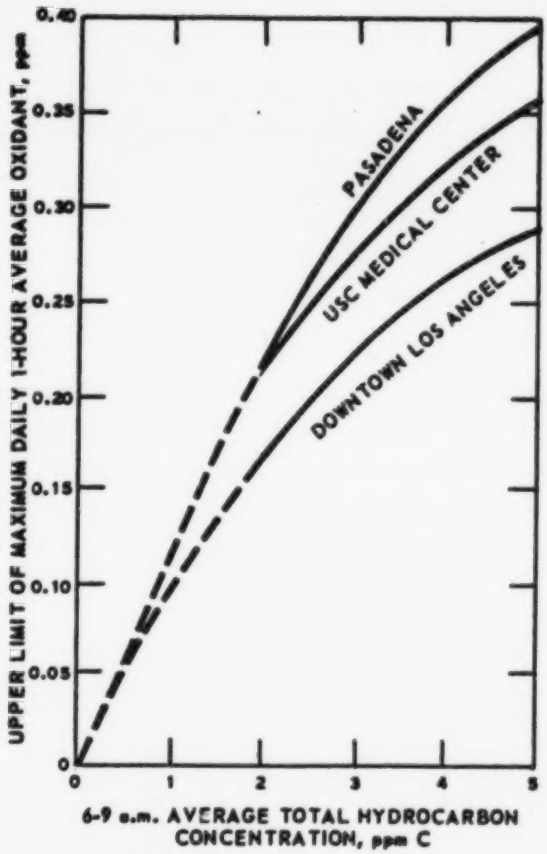

Figure 5. Upper limit of maximum daily oxidant at three Los Angeles County stations, May through October 1967[3]

is a weakness of this technique. This method assumes that hydrocarbon concentrations are linearly related to emissions and that oxidant concentrations are linearly related to hydrocarbon concentrations, and hence to hydrocarbon emissions. Alternatively, under the nonlinear assumption, one could use the upper-limit curve depicted in Figure 1 or the Appendix J relationship to determine the impact of an increase or decrease in hydrocarbon emissions on oxidant levels.

Curves other than those shown so far have been put forth for specific cities. These city-specific relationships are an improvement for the individual locations to which they are applied; the curves shown thus far are composites made up of data from a number of urban areas. They are also based on data taken before the EPA reference method (chemiluminescence) for oxidant was defined. Preparation of city-specific curves based on more recent data would thus likely improve the predictive capability of this method due to the methodological and locational compatibility of measurements.

Figure 6 shows the difference between the upper-limit curve of Figure 1 and a curve based solely on data for Denver.[3] In all cases, peak oxidant levels in Denver are greater, for a given hydrocarbon concentration, than would be estimated from the composite curve. These curves are based on concentrations of <u>total</u> hydrocarbons.

Figure 7 shows similar relationships for Los Angeles[1] based on <u>non-methane</u> hydrocarbons and the upper-limit curve of Figure 2. Again, Los Angeles experiences higher peak oxidant levels for a given level of hydrocarbons up to oxidant concentrations of about 0.22 ppm. Not every city would, of course, experience concentrations higher than those demonstrated by the composite curves.

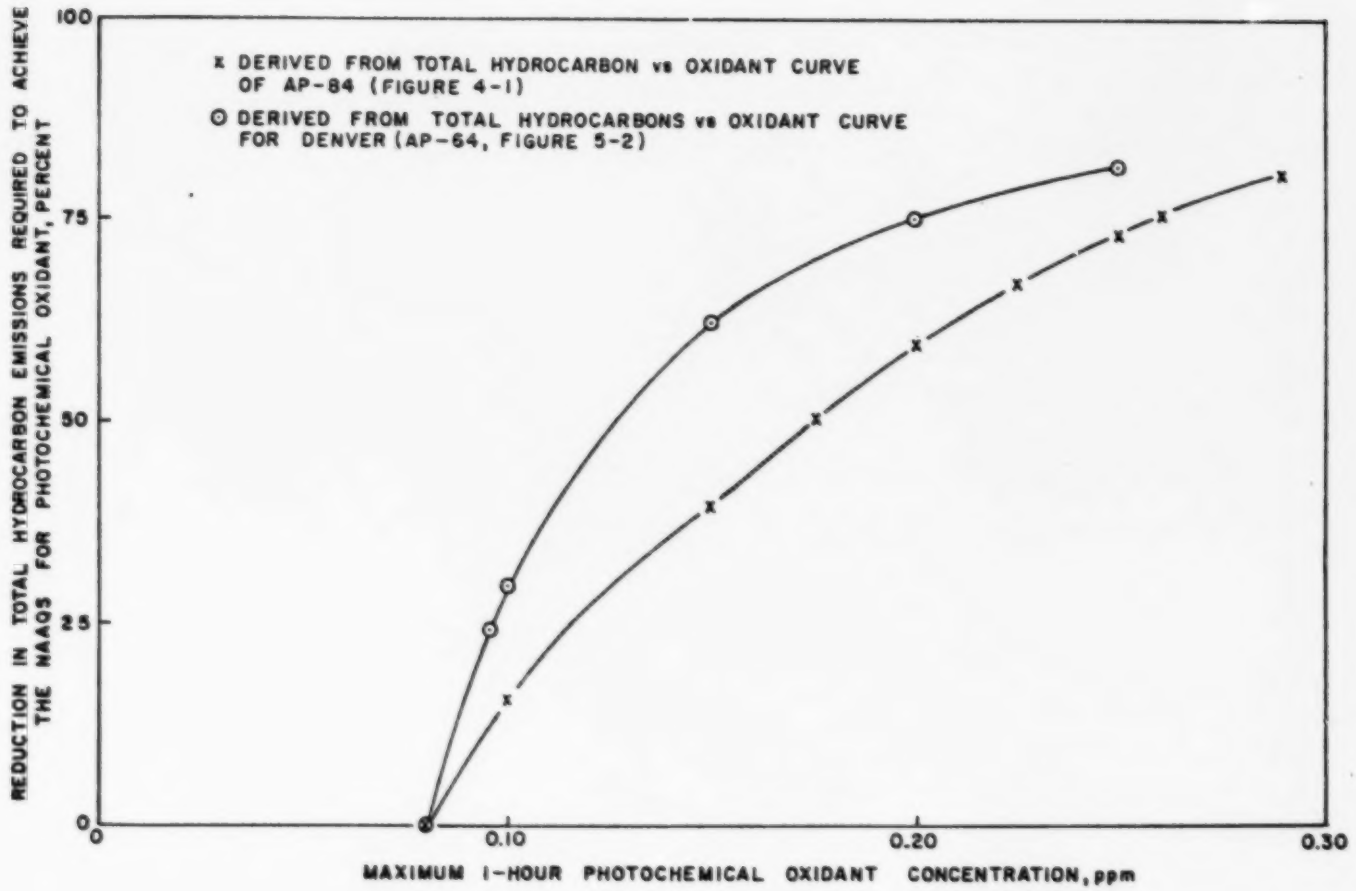
x DERIVED FROM TOTAL HYDROCARBON vs OXIDANT CURVE OF AP-84 (FIGURE 4-1)
⊙ DERIVED FROM TOTAL HYDROCARBONS vs OXIDANT CURVE FOR DENVER (AP-64, FIGURE 5-2)
REDUCTION IN TOTAL HYDROCARBON EMISSIONS REQUIRED TO ACHIEVE THE NAAQS FOR PHOTOCHEMICAL OXIDANT, PERCENT
100
75
50
25
0
0
0.10
0.20
0.30
MAXIMUM 1-HOUR PHOTOCHEMICAL OXIDANT CONCENTRATION, ppm

Figure 6. Comparison of total hydrocarbon versus oxidant curve of AP-84 with curve for Denver

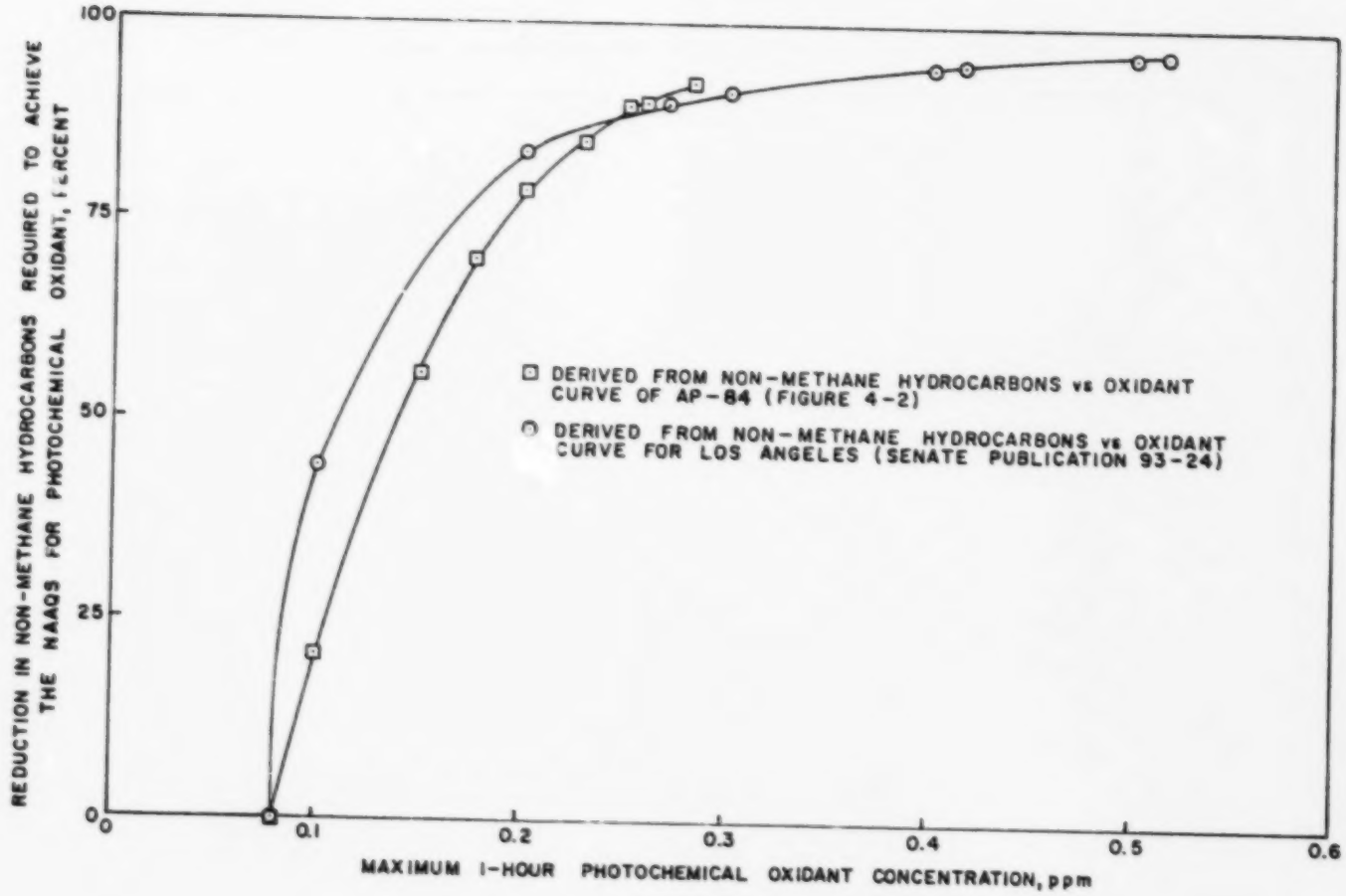

Figure 7. Comparison of nonmethane hydrocarbons versus oxidant curve of AP-84 with curve for Los Angeles

In developing a city-specific curve it is important to have sufficient data to define the upper-limit curve clearly, since the data points defining this curve generally occurs infrequently.

LIMITATIONS

The assumptions that must be made in using a proportional model for predicting expected maximum oxidant concentrations were discussed at the beginning of this section. These assumptions become even more tenuous when trying to predict concentrations of a secondary pollutant nonlinearly related to its precursors, than when trying to predict concentrations of a relatively stable pollutant like carbon monoxide. It should be remembered that this technique is useful only for providing an indication of what concentrations may result from a change in emissions of hydrocarbons. It does not consider the dependence of oxidants on the hydrocarbon-nitrogen dioxide ratio.

The Appendix J relationship is independent of city size, although this problem can be accommodated by the development of a location-specific curve. The fact that the Appendix J type relationship depends heavily on monitor location also indicates the advantage of using location-specific relationships.

SPECIAL FEATURES

This technique is relatively inexpensive and easy to apply, requiring perhaps 1 man-week more than the previous technique when a location-specific upper-limit curve is prepared for the 6 to 9 a.m. average hydrocarbons, maximum daily 1-hour average oxidant concentration relationships. This is also the first technique to be considered thus far which attempts to describe the nonlinear relationship between oxidant and oxidant precursor concentrations, based on empirical data. It thus also comes closer to modeling adequately the expected peak oxidant concentrations.

REFERENCES

1. Air Quality and Automobile Emission Control, Volume 3. The Relationship of Emissions to Ambient Air Quality. U.S. Senate, Committee on Public Works, Serial No. 93-24. September 1974.

2. Air Quality Criteria for Nitrogen Oxides. U.S. Environmental Protection Agency. Report AP-84. January 1971.

3. Air Quality Criteria for Hydrocarbons. U.S. Environmental Protection Agency. Report AP-64. March 1970.

SECTION V

GIFFORD-HANNA PHOTOCHEMICAL MODEL

For the past several years F. A. Gifford and S. R. Hanna of the Atmospheric Turbulence and Diffusion Laboratory (ATDL) at Oak Ridge, Tennessee have been active in the development and validation of simple methods for estimating pollutant concentrations in urban areas. Much of their effort had been restricted to the analysis of chemically inert pollutants, but they have recently generalized their model to treat pollutants undergoing photochemical reactions.

APPLICABILITY AND RELIABILITY

The Gifford-Hanna model is basically a "box model" in which average pollutant concentrations within the box are taken to be proportional to the ratio of the average area source strength to the wind speed. The proportionality constant is set equal to the average width of the region divided by the average depth of the pollutant cloud over the area. This depth is allowed to vary as a function of atmospheric stability, and it may be calculated by integrating the Gaussian plume model over the extent of the area source.

For purposes of chemical kinetics calculations the pollutant concentrations are assumed to be uniform within the volume defined by the area of the region and the depth of the pollutant cloud. By nondimensionalizing the concentrations which appear in the equations governing chemical reactions, it is possible to gain some insight into the importance of a particular reaction upon the concentration of a particular species. For

instance, if the steady state nondimensionalized concentration of a particular substance is close to unity, it is possible to neglect chemical transformation for the associated meteorological conditions and emission rates.

The Gifford-Hanna model is intended to be applicable to any location, although published reports of its reliability describe experience with the model only in Los Angeles and Denver. Table 3 displays results in Los Angeles.[1] The ozone concentrations were not given in reference 1; observed values of ozone (and the other pollutants) were obtained from reference 2, while calculated concentrations were derived from the relationship:[1]

$$\left[O_3\right] = 2\left[NO_2\right]/\left[NO\right] \text{ pphm} \qquad (15)$$

Calculated concentrations of NO_2 and NO were used to determine O_3 concentrations, with a correlation coefficient of 0.84 between calculated and observed ozone levels. Ozone concentrations were also calculated using observed NO_2 and NO concentrations, and the correlation coefficient is 0.97. Both of these are significant at better than the 2 percent level.

While each of these correlation coefficients is significant, the question arises as to the utility of predicting areal average concentrations for a large region. Also, although the calculated and observed values correlate well, the "calibration factor," or the ratio of observed to calculated concentrations becomes progressively greater as the morning progresses and higher ozone concentrations are observed. The observed concentration is almost ten times that calculated at noon.

Similar results were obtained in an application of the ATDL model to Denver, Colorado,[3] as presented in Table 4. In this case, concentrations were compared hourly at five locations. Again, the correlation between observed and calculated ozone concentrations is good, but the ATDL model underpredicts severely during peak hours.

Table 3. COMPARISON OF OBSERVED HOURLY REGIONAL AVERAGE CONCENTRATIONS OF RH, NO_2, NO, AND O_3 WITH CONCENTRATIONS PREDICTED BY THE GIFFORD-HANNA ATDL MODEL FOR LOS ANGELES, SEPTEMBER 30, 1969

	RH (ppm)		NO_2 (pphm)		NO (pphm)		O_3 (pphm)		
Hour	CALC	OBS	CALC	OBS	CALC	OBS	CALC[a]	OBS	CALC[b]
0600	7	7	6	6	33	33	0.36	1	0.36
0700	7	7	8	10	23	30	0.70	2	0.67
0800	6	4	7	17	14	22	1.00	4	1.55
0900	4	4	6	18	9	11	1.33	6	3.27
1000	3	4	4	14	7	4	1.14	9	7.00
1100	2	4	3	11	5	3	1.20	12	7.33
1200	2	5	3	15	4	4	1.50	14	7.50
	r = 0.55		r = 0.05		r = 0.97		r = 0.84[a] r = 0.97[b]		

[a] $[O_3] = 2[NO_2]/[NO]$ using calculated concentrations.

[b] $[O_3] = 2[NO_2]/[NO]$ using observed concentrations.

Table 4. COMPARISON OF OBSERVED HOURLY AVERAGE CONCENTRATIONS OF O_3, HC, AND CO WITH CONCENTRATIONS PREDICTED BY THE GIFFORD-HANNA ATDL MODEL AT FIVE LOCATIONS IN DENVER, COLORADO, AUGUST 13, 1973

Station	Hour	O_3 ($\mu g/m^3$)		HC ($\mu g/m^3$)		CO (mg/m^3)	
		Calc	Obs	Calc	Obs	Calc	Obs
A	0600	26.7	29			2.3	2.3
	0700	28.3	59			21.0	1.1
	0800	29.8	84			6.23	1.1
	0900	31.0	-			3.95	3.4
	1000	31.9	167			5.57	3.4
	1100	32.8	274			3.63	3.4
	1200	33.8	382			4.54	3.4
C	0600	26.7	39	2394	2394	2.3	2.3
	0700	28.3	59	21615	1862	21.0	3.4
	0800	29.8	98	6358	1729	6.23	2.3
	0900	31.0	118	3988	1995	3.95	2.3
	1000	31.9	225	5562	2128	5.57	2.3
	1100	32.8	323	3589	2128	3.63	3.4
	1200	33.8	421	4439	2394	4.54	4.6
D	0600	26.7	29	1862	1862	4.0	4.0
	0700	28.3	59	16812	2261	36.5	5.7
	0800	29.8	176	4945	3059	10.8	5.7
	0900	31.0	118	3102	1995	6.87	5.7
	1000	31.9	-	4326	1862	9.68	6.9
	1100	32.8	235	2791	1795	6.31	6.9
	1200	33.8	304	3452	1729	7.89	5.7
E	0600	26.7	65	1197	1197		
	0700	28.3	-	10807	1197		
	0800	29.8	78	3179	1130		
	0900	31.0	98	1994	1130		
	1000	31.9	114	2781	1130		
	1100	32.8	147	1794	1197		
	1200	33.8	235	2219	1463		
F	0600	26.7	-	1596	1596	3.4	3.4
	0700	28.3	49	9607	1463	20.7	3.4
	0800	29.8	65	12716	1729	27.6	4.6
	0900	31.0	127	10636	1729	23.4	5.7
	1000	31.9	255	7416	1862	16.5	5.7
	1100	32.8	314	5981	1729	13.4	5.7
	1200	33.8	216	7891	1463	1..9	4.6
		r = 0.85		r = 0.14		r = 0.22	

Based on these results, it is evident that the Gifford-Hanna model might predict trends in ozone concentrations reasonably well, but it seriously underpredicts amounts of ozone, especially at higher concentrations.

DATA AND MANPOWER REQUIREMENTS

The data requirements for using the Gifford-Hanna model are basically the reactive hydrocarbon (assumed to be propylene) emission density, the early morning (6 a.m.) concentrations of NO and NO_2, and hourly wind speed values. If the emission densities of NO and NO_2 are known they may be used, although in application[1,4] it has been assumed that $Q_{NO} = 0.3\ Q_{RH}$ and $Q_{NO_2} = 0.2\ Q_{RH}$, and hence $Q_{NO} = 1.5\ Q_{NO_2}$. It is also assumed that at 6 a.m. $Q_{NO_2}/Q_{NO} = [NO_2] / [NO]$, so that all that is required is the reactive hydrocarbon emission density and the 6 a.m. NO_2 concentration to determine the remaining parameters.

The emissions data have been gridded in applications of the model, and 8 miles squared[1,3] and 8 km squared[4] grids have been used. The choice of grid size seems to be up to the user; no guidance or specification has been given. For areal average concentrations, average emissions for a whole region could be used.

The additional manpower necessary to run this model, compared to the models previously discussed in this report, is about 1 man-week to collect the wind data and make the concentration calculations.

APPLICATION OF THE TECHNIQUE

The simple Gifford-Hanna ATDL model for nonreactive pollutants calculates surface concentrations $[C]$ as being proportional to the local source strength divided by the wind speed:

$$[C] \sim Q/U. \qquad (16)$$

The photochemical model is an extension of this simple relationship to include chemically reactive pollutants.

The reaction scheme in this model was originally proposed by Friedlander and Seinfeld[5] and consists of the following four equations:

$$\frac{\partial}{\partial t}\left[NO_2\right] = \left[NO_2\right]\left[RH\right]\left(\alpha\left[NO\right] - \lambda\left[NO_2\right]\right) \tag{17}$$

$$\frac{\partial}{\partial t}\left[NO\right] = -\alpha\left[NO_2\right]\left[NO\right]\left[RH\right] \tag{18}$$

$$\frac{\partial}{\partial t}\left[RH\right] = -\left[NO_2\right]\left[RH\right]\left(\theta + \frac{\mu}{\left[NO\right]}\right) \tag{19}$$

$$\left[O_3\right] = \beta\frac{\left[NO_2\right]}{\left[NO\right]} \tag{20}$$

where $\alpha = \frac{1}{600}$ ppm^{-2} sec^{-1}

$\mu = \frac{1}{2.4 \times 10^5}$ sec^{-1}

$\theta = \frac{1}{3 \times 10^4}$ ppm^{-1} sec^{-1}

$\lambda = \frac{1}{3 \times 10^3}$ ppm^{-2} sec^{-1}

$\beta = 0.02$ ppm

The concentrations in equations (17) through (20) are indicated in brackets. No functional dependence with solar radiation intensity is specified for

these reaction rates. Equations (17), (18), and (19) are nondimensionalized for performing the actual calculations; nondimensionalized concentrations $\left[C\right]^*$ and times t^* may be found from the following transformation:

$$\left[C\right]^* = \frac{\left[C\right] uz}{Q\ \Delta x} \tag{21}$$

$$t^* = \frac{t\ u}{\Delta x} \tag{22}$$

where $\Delta x = A\ Z$

u = wind speed (m/sec)

Q = emission density ($cm^3\ m^{-2}\ s^{-1}$)

The parameter $A = \Delta x/Z$ is a function of stability and equals 50, 200, or 600 m for unstable, neutral, and stable conditions.[1]

Two approaches are possible for the prediction of ozone levels. The first option is to assume that the process has reached a steady state so that the time derivative on the left side of the equations can be set to zero. The equations may then be solved algebraically for the nondimensionalized concentrations. These can then be redimensionalized and compared with measured values. Since the steady state approximation may not strictly be applied due to the time variation of emission density and solar radiation intensity, it is open to some question which hour should be chosen for the comparison of measured and "steady state" values. In his Los Angeles validation study,[1] Hanna picked the noon hour for a comparison.

The second way in which the model may be applied is to solve the chemical kinetics equation numerically by use of a Runge-Kutta technique to obtain values for nondimensionalized concentrations as a function of time. If an hour such as 6:00 a.m. is chosen as the time when all nondimensionalized concentrations are equal to 1.0, then the time variation of the wind speed

and nondimensionalized concentrations may be used to project actual concentrations from their 6:00 a.m. values.

Dimensionalized concentrations are computed from their nondimensionalized form by assuming that source strengths and stability are constant and that equation (2) holds at 6:00 a.m.:

$$[C] = \frac{u_6}{u} [C]^* [C]_6 \qquad (23)$$

where u = wind speed (m/sec)

u_6 = wind speed at 6:00 a.m. (m/sec)

$[C]^*$ = nondimensionalized concentration

$[C]_6$ = concentration at 6:00 a.m.

Ozone concentrations are found using equation (20).

LIMITATIONS

A major limitation of this technique is that although it predicts trends in ozone concentrations well during the day, it predicts actual concentrations poorly, especially as they build up during the day. A second limitation is that it assumes that ozone concentrations depend only on the ratio of NO_2 to NO concentrations, when they have been shown[6] to be a function of hydrocarbon concentrations also. This dependence is treated indirectly in the ATDL model by the dependence of NO_2 and NO concentrations on reactive hydrocarbon concentrations and emissions in equations (17), (18), and (19). However, the assumption is still made that predicted ozone concentrations are directly proportional to the accurately predicted concentration ratios of NO_2 to NO. The last column of Table 3 shows that ozone concentrations are not well predicted by this ratio, even when using measured values of NO_2 and NO.

The grid element scale is somewhat limiting to spatial location of peak ozone values. This can be accommodated to some degree by making the grid elements smaller. However, this presents two further problems. The first is that the smaller grid size allows even less time for the development of the photochemical reactions. Including pollutant transport from a number of upwind grids will help this situation somewhat, but a computer must be used to handle the data efficiently, and this technique features the lack of computer requirements.

SPECIAL FEATURES

The Gifford-Hanna model marks a transition point. It is the last of the models considered here which does not require a computer, while it is the first to be considered which attempts to model photochemical reaction mechanisms. It also includes explicit consideration of the meteorological parameters of wind speed and stability. Although the model fails to predict concentrations of ozone adequately, it could be useful for examining trends in concentrations. An additional application of the model has been in determining "critical" wind speeds below which photochemical smog will be a problem in a region.[1]

REFERENCES

1. Hanna, S. R. A Simple Dispersion Model for the Analysis of Chemically Reactive Pollutants. Atmospheric Environment. Pergamon Press. 7:803-817. 1973.

2. Sklarew, Ralph C., Allan J. Fabrick, and Judith E. Prager. Mathematical Modeling of Photochemical Smog Using the PICK Method. JAPCA. 22(11):865. November 1972.

3. Photochemical Oxidant Modeling: Detailed Technical Report. GCA/Technology Division, GCA-TR-75-11-G(2), Draft Final Report - Volume II. April 1975.

4. Hanna, S. R. Application of a Simple Model of Photochemical Smog. 3rd Clean Air Congress of the International Union of Air Pollution Prevention Associations, Dusseldorf, Germany. October 8-12, 1973.

5. Friedlander, S. K. and J. H. Seinfeld. A Dynamic Model of Photochemical Smog. Environmental Science and Technology. 3:1175-1181. 1969.

6. Schuck, et al. Relationship of Hydrocarbons to Oxidants in Ambient Atmospheres. JAPCA, 20(5):297. May 1970.

SECTION VI
STATISTICAL RELATIONSHIPS: REPRO-MODELING

Another technique for relating highway system changes to resulting oxidant levels is the derivation of statistical relationships between the important independent variables (emissions of hydrocarbons and NO_x, meteorology, temporal, and spatial effects) and the dependent variables (peak hourly-averaged oxidant concentrations) in an "input-output" model. Development of such models is underway within EPA, although proven techniques are not yet available.

One statistical technique which has been successfully applied to oxidant concentration prediction is repro-modeling, and the remainder of this section will deal with this approach.

A repro-model is a "model of a model" which seeks to provide an approximation to a more complex model. The development of a repro-model focuses on relationships between (some) input and output variables of the complex model, and the repro-model itself is a "fit" to these relationships. Strong points of repro-models are computation times that may be orders of magnitude less than those of the complex models on which they are based, much greater ease of application because of reduced input data requirements and overall complexity, and the opportunity to make many more applications of the model, for example, to strategies analysis for policy planning. The major drawbacks to repro-models are first, that since they are "models of models" they are no better than the basis models, and second, that a repro-model may produce only a portion of the picture available from the basis model. This latter point is

due to the fact that only selected input and output variables are chosen on which to build the repro-model, such as the relationship of peak ozone levels to emissions, with other variables held constant.

APPLICABILITY AND RELIABILITY

Repro-modeling has been applied to diverse topics including freeway on-ramp control, radar cross section determination, and photochemical diffusion processes. A repro-model has been built for the Systems Applications, Inc. photochemical advection/diffusion model. This repro-model is based on 100 runs of the SAI model for the Los Angeles basin. One of these runs used input variables obtained for September 30, 1969, a day on which high oxidant levels were observed and which was included in a previous calibration of the SAI model. Several inputs were then varied in each of the remaining 99 runs. More specifically, five aggregate input variables were used. These were (1) mobile source NO_x, (2) mobile source hydrocarbons, (3) fixed source hydrocarbons, (4) NO_x initial values, and (5) hydrocarbons initial values. Each of these independent input variables was expressed as a percentage of the values of the base case test day. Twelve outputs were examined: (1) the peak 1-hour average oxidant concentration in the Los Angeles basin, (2 to 9) the peak 1-hour average concentration at each of eight specific locations in the basin, and (10 to 12) 10-hour average concentrations of NO_2 at three specific locations. The overall repro-model was made up of 12 repro-models, each of which related the five independent variables to one of the dependent variables. Ninety of the 100 runs of the SAI model were used to build the repro-models; the other 10 were used for independent testing of the resulting model. Details of the development and specific functional forms of this repro-model are discussed in reference 1. A more general description of repro-modeling is presented in reference 2.

It should be noted that the repro-model described in reference 1 of this section has the following limitations to its applicability: (1) the original (SAI) model on which it is based was calibrated for Los Angeles only, (2) the meteorological inputs remained constant, (3) other inputs to the SAI model remained fixed, such as the distribution of traffic, and (4) the repro-model is applicable only so far as the SAI model is applicable. This single instance to date of repro-modeling of a complex photochemical diffusion model has developed relationships between emissions of NO_x and hydrocarbons and resulting oxidant and NO_2 concentrations. It is strictly applicable only to investigating the effects of changing the magnitude of emissions under the conditions that were obtained in the Los Angeles basin on September 30, 1969. It is also useful, however, for determining the direction and relative magnitude of concentration changes for varying emissions. Other repro-models could be developed from different inputs and outputs of the SAI model, to investigate the effects of different emissions distributions, for example. None of these repro-models would be more reliable than the SAI model on which they are based.

DATA AND MANPOWER REQUIREMENTS

The extensive data and manpower requirements occur during the development of the repro-model. They would be greater than those listed in Section IX of this report which describes the application of the SAI areawide model.

A main reason for repro-models is the great reduction in manpower and data needed to run them compared to the requirements of the complex, basic model. The repro-model of the SAI model applied to the Los Angeles basin requires only five input parameters:

- Percentage of test day mobile source NO_x emissions
- Percentage of test day mobile source hydrocarbon emissions
- Percentage of test day fixed source hydrocarbon emissions

- Percentage of test day initial conditions for NO_x
- Percentage of test day initial conditions for hydrocarbons

For this case the test day used for constructing the repro-model was September 30, 1969. The repro-model may be used to investigate the effects of alternate emission reduction strategies on oxidant and NO_2 concentrations relative to the test day. Absolute values of emissions need not be known, except if required to determine them as a percentage of the test day emissions on which the repro-model is based. Thus, the manpower and data requirements, and the computer costs, are relatively small. The development of the repro-model described in this section required about 2 man-weeks to decide upon the input variable changes for the SAI model runs and about 1 man-week for building the repro-model.[3] It is emphasized, however, that these manpower figures exclude the effort in calibrating the SAI model and running the 100 cases. (The SAI model is discussed in Section IX.)

APPLICATION OF THE TECHNIQUE

As discussed previously, the largest effort involved in repro-modeling occurs during the actual model development. This step will not be described here; discussions on building repro-models are available elsewhere.[1,2] Once a repro-model is built, it is easy to apply.

The repro-model constructed for Los Angeles has specific application to transportation control policy evaluation. Demonstrations of its use have been to assess the impact on oxidant levels of motor vehicle emission controls, and the effects of a 1-day VMT reduction. These two examples of use were accomplished by changing the emissions inputs relative to the 1969 base case values. The model input changes and the model outputs for these two examples are shown in Tables 5 and 6.

Table 5. IMPACT OF FEDERAL EMISSION CONTROL STANDARDS MOBILE SOURCES[a] — OXIDANT (in pphm)

Year	NO_x mobile[b] source em.	HC mobile source em.	Grid location[c]								
			Peak	10,24	10,21	15,20	20,20	7,17	12,17	25,13	12,9
1969	100	100	45	45	25	30	16	3	14	16	2
1970	103	90	40	40	21	26	13	2	11	12	1
1971	102	78	33	33	15	21	10	2	7	10	1
1972	95	65	25	25	8	15	6	2	2	7	1
1973	81	53	17	17	4	9	3	2	2	4	1
1974	65	45	11	11	3	5	3	2	2	4	1
1975	54	35	7	5	3	3	3	2	2	3	1
1976	42	25	7	3	2	3	3	2	1	3	1
1977	33	18	7	2	2	2	2	2	1	2	0
1978	27	15	7	2	2	2	2	3	1	2	0
1979	22	12	7	2	2	2	2	3	1	2	0

[a]Vehicle miles of travel held at 1969 level.

[b]Fixed source hydrocarbons held at 100 percent. All initial conditions set at values typical for the mobile source emission control policy.

[c]Refers to grid overlay of the Los Angeles basin employed in the SAI model. See Section IX.

Source: Reference 1.

Table 6. EFFECTS OF SINGLE DAY TRAFFIC REDUCTION POLICY ON AIR QUALITY (OXIDANT, pphm)

Zone	Baseline[a]	20% reduction in mobile Source emissions[b]	50% of baseline[c]	20% reduction of mobile source emissions from 50% base[d]
Peak	45	37	7	7
10,24	45	37	6	4
10,21	25	20	3	3
15,20	30	25	4	3
20,20	16	13	3	3
7,17	3	3	2	2
12,17	14	11	2	1
25,13	16	14	3	3
12, 9	2	1	1	2

[a]Policy: 100,100,100,100,100 (NOx and HC mobile source emissions, HC fixed source emissions, and NOx and HC initial condition, respectively.)

[b]Policy: 80,80,100,100,100

[c]Policy: 50, 50, 50, 69, 50. The 69% value of NOx initial condition variable results from the uncontrolled NOx fixed sources.

[d]Policy: 40,40,50,69,50

Source: Reference 1.

The user of the repro-model is not completely free to vary the input values without bound. Valid input changes are constrained by the input and output values used to build the model. Table 7 shows the constraints for the Los Angeles model.

LIMITATIONS

The basic limitation to the repro-modeling approach is that the repro-model is a functional representation of the inputs and outputs of another, more complex basis model. The repro-model will reproduce the results of the basis model, but it will not produce results which are closer to reality. Also, the repro-model incorporates only a portion of the input and output variables of the basis model, restricting its applicability to specif... conditions. For the Los Angeles case, the only changeable variables are magnitudes of NO_x and hydrocarbon emissions. Spatial variation cannot be modeled, nor can changes in meteorological parameters. A final limitation to the use of repro-models, as opposed to the repro-modeling technique, is that at present there exists only the model for Los Angeles. Application to other locations depends on the application and calibration of one of the photochemical diffusion models discussed in following sections to these other locations.

SPECIAL FEATURES

The fact that a complex photochemical diffusion model must be calibrated for a location before a repro-model can be built raises the question of why develop the repro-model at all when the basis model is available. The answer to this question derives from a major feature of repro-modeling – the low cost and ease of operation compared to the basis model. For locations lacking the resources to continually apply the complex basis model, a repro-model could be developed, based on careful considerations of inputs and outputs in light of potential decision-making applications, which could then be used repeatedly to assess air

Table 7. INPUT VARIABLE CONSTRAINTS

$x_1 + x_2 > 30$	(1)
$x_1 + x_2 < 240$	(2)
$x_1 - x_2 < 40$	(3)
$-x_1 + x_2 < 20$	(4)
$x_2 > 0$	(5)
$x_3 > 0$	(6)
$x_3 < 100$	(7)
$x_4 - 0.558x_1 > 29.2$	(8)
$x_4 - 0.682x_1 < 46.8$	(9)
$-x_5 + 0.756x_2 + 0.144x_3 < 5$	(10)
$x_5 - 0.924x_2 - 0.176x_3 < 5$	(11)
$x_5 > 0$	(12)

x_1 = % of test day's mobile source NOx emissions

x_2 = % of test day's mobile source hydrocarbon emissions

x_3 = % of test day's fixed source hydrocarbon emissions

x_4 = % of test day's initial and boundary conditions for NOx

x_5 = % of test day's initial and boundary conditions for hydrocarbons

Source: Reference 1.

quality impacts. Even if adequate resources are available to apply a complex model repeatedly, in most instances it would be more cost effective to use repro-models for repeated applications.

REFERENCES

1. Horowitz, Alan, Meisel, William S., and David C. Collins. The Application of Repro-Modeling to the Analysis of a Photochemical Pollution Model. Technology Service Corporation Report, prepared for Office of Research and Development, USEPA, Washington, D.C. December 1973.

2. Meisel, William S., and David C. Collins. Repro-Modeling: An Approach to Efficient Model Utilization and Interpretation. IEEE Transactions on Systems, Man, and Cybernetics. Vol. SMC-3. No. 4. July 1973.

3. Teener, M. D., Technology Service Corporation, Santa Monica, California. Personal Communications.

SECTION VII

REACTIVE ENVIRONMENTAL SIMULATION MODEL

INTRODUCTION

The Reactive Environmental Simulation Model (REM) is the first of three large computer models described in this report. Each of these models is based on the general form of the mass conserving advection/diffusion equation:

$$\frac{\partial C_i}{\partial t} + u\frac{\partial C_i}{\partial x} + v\frac{\partial C_i}{\partial y} + w\frac{\partial C_i}{\partial z} =$$

$$\frac{\partial}{\partial x}\left(K_x\frac{\partial Ci}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y\frac{\partial Ci}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_z\frac{\partial Ci}{\partial z}\right) + R_i + S_i \qquad (24)$$

The mean concentration of pollutant species i is given by C_i; u, v, and w are the horizontal and vertical wind components; K_x, K_y, and K_z are the horizontal and vertical eddy diffusivities; and R_i and S_i are the average reaction and emission rates for the i^{th} species.

The REM and DIFKIN (described in the following section) models are trajectory models based on a Lagrangian or moving coordinate system. A vertical air column moves along a trajectory determined by the horizontal wind components. Pollutant concentrations are assumed to be homogeneous horizontally in the air column, and vertical advection and horizontal diffusion are ignored, so that equation 24 becomes:

$$\frac{\partial c_i}{\partial t} = \frac{\partial}{\partial z}\left(K_z \frac{\partial c_i}{\partial z}\right) + R_i + S_i \qquad (25)$$

The REM model makes a further simplifying assumption regarding vertical diffusion. It considers the effect of vertical diffusion to be solely the production of a homogeneous concentration of pollutants in the vertical from the ground to the mixing height. Pollutant concentrations within the column of air thus depend upon the emission of pollutants into the column, productive and destructive photochemical reactions, and the mixing height. Hence, equation (25) becomes:

$$\frac{\partial c_i}{\partial t} = S_i + R_i + H_i \qquad (26)$$

where H_i is the rate of change of the concentration of pollutant i due to variation in the mixing height.

Changes in mixing height occur from changes of the base elevation due to changing topography, while changes in the elevation of the top of the mixing height are computed as functions of the air temperature at the ground. The effects of changes in volume of the air column due to mixing height fluctuations (the base area is constant) on pollutant concentrations within the column are the following.[1] If the columnar volume increases the concentrations decrease to conserve mass. If, on the other hand, the volume decreases, the concentration is assumed to remain constant while part of the mass (proportional to the volume decrease) is assumed to be lost through the top of the column.

Under the assumptions expressed in equation (26) the REM model treats the column of air as a moving smog chamber which has a variable volume and the capacity for fresh contaminant input during irradiation.

Consistent with this treatment, emphasis is placed on adequately describing the reaction mechanisms occurring during photochemical smog formation as derived from irradiation chamber data. REM uses a more detailed

chemical kinetics scheme than either the DIFKIN or Areawide models to be discussed in subsequent sections. Table 8 presents the chemical reactions and their respective rates included in REM. These can be compared with the reaction schemes presented in later sections of this report.

Because of the important dependence of concentrations on the mixing height of the air column relative to the ground elevation, REM computes mixing heights along the trajectory. This is accomplished using the standard technique of intercepting the morning or afternoon sounding data with the dry adiabatic lapse rate from the surface temperature.

The trajectory of the air column is calculated by inverse distance squared weighting of wind velocity data from reporting meteorological stations. The individual components of wind velocity from each station are divided by the square of the station distance from the air column; these are summed, and multiplied by the sum of the squares of the distances.

This introduction has outlined the major points of the REM model. More details regarding the development of the model and the specific calculational procedures may be found in references 1 and 2.

APPLICABILITY AND RELIABILITY

REM was designed around a photochemical reaction scheme built to replicate smog chamber data as closely as practicable. The smog chamber simulation was then extended to the atmosphere under the assumptions on advection and diffusion previously discussed: a Lagrangian, or moving, coordinate system is attached to a column of air with a fixed base area and a height which varies with topography and the atmospheric mixing height, and in which pollutant concentrations are homogeneously mixed.

Table 8. CHEMICAL DYNAMICS MODULE FOR REM[2]

	Reaction		Rate (ppm^{-1} min^{-1})
1	NO2+HV	= NO + O	4×10^{-1}
2	O+O2+M	= O3 + M	1.4×10^{6}
3	O3+NO	= NO2 + O2	4×10^{-1}
4	NO2+O3	= NO3 + O2	1×10^{-5}
5	C2H3O3 + O2	= C2H3O2 + O3	2×10^{1}
6	NO3 + NO	= 2NO2	2.45×10^{2}
7	C3H6 + OH	= CH3CHO + CH3	1×10^{3}
8	NO + HO2	= NO2 + OH	1×10^{1}
9	H + O2 + M	= HO2 + M	1×10^{6}
10	C2H3O + O2	= C2H3O3	1×10^{5}
11	NO2 + OH	= HNO3	1×10^{2}
12	OH + O3	= HO2 + O2	1×10^{1}
13	OH + CO	= H + CO2	3×10^{0}
14	CH3 + O2 + M	= CH3O2 + M	1.4×10^{6}
15	CH3O2 + NO	= CH3O + NO2	2×10^{0}
16	CH3O + O2 + NO	= CH3O2 + NO2	1×10^{1}
17	C2H3O3 + NO	= C2H3O2 + NO2	2.5×10^{0}
18	C2H3O2 + NO	= C2H3O + NO2	2×10^{1}
19	C2H4O2 + NO	= CH3CHO + NO2	1×10^{2}
20	CH3O + O2	= HCHO + HO2	2×10^{2}
21	C3H6 + O	= CH3 + C2H3O	3.5×10^{1}
22	C3H6 + O3	= HCHO + C2H4O2	5×10^{-5}
23	C3H6 + O + O2	= HCHO + C2H4O2	1.75×10^{1}
24	C2H4O2 + O2	= C2H3O3 + OH	3×10^{2}
25	C3H6 + HO2	= CH3O + CH3CHO	1×10^{0}
26	C3H6 + MEO2	= CH3 + MEO + C2H3O	1×10^{-2}
27	C2H3O + M	= CH3 + CO + M	1×10^{1}
28	CH3O + NO2	= CH3ONO2	1×10^{0}
29	C2H3O3 + NO2	= C2H3O3NO2	2×10^{-1}
30	DUMHC + O	= CH3 + C2H3O	7×10^{0}
31	HCHO + HV	= H + H + CO	3×10^{-3}
32	NO2 + NO3 + H2O	= HNO3 + "	1×10^{2}

The trajectory of the air column is determined by inverse distance squared weighting of wind speed and direction data from reporting stations. So far as the assumptions made in building REM are plausible the model should be applicable. The suppression of a more thorough description of atmospheric transport and diffusion of the pollutant species, at least for Los Angeles, is based on field study data[3] of pollutant concentrations as a function of altitude over Los Angeles.

In theory, the model could be applied to any location having sufficient data to make the trajectory and mixing height calculations. The trajectory could be computed using data from one meteorological station, although the accuracy improves substantially with an increasing number of stations. The availability of temperature sounding data to use in mixing height calculations is somewhat limited, although such data are available for a number of urban areas. These data are routinely taken by the National Weather Service, and historical records are maintained at the National Climatic Center in Asheville, N. C. The model does, however, allow for direct input of estimated mixing heights should lack of data preclude their calculation.

Application of REM to highway system evaluation would involve making a number of model runs for different trajectories to develop sufficient detail. This involves trajectories for different end points, for spatial detail, and different ending times, for temporal detail to ensure that highest values are determined. The end point and time of the trajectory are basic inputs to the model, so that it is relatively simple to specify exactly the locations to be modeled.

REM has been tested only in Los Angeles. The results of the validation runs are summarized as follows:[1]

- CO, less than a factor of 2 in more than 80 percent of the comparisons; 40 percent agreement within one part per million.

- O_3, within a factor of 2, 75 percent of the comparisons.
- NO, within a factor of 2, 75 percent of the comparisons; 90 percent agreement within 0.02 ppm.
- NO_2, within a factor of 2, 60 percent of the comparisons.

These comparisons are between instantaneous predicted values on the half hour and the average observed concentration for the hour. The model has not yet been tested in other cities.

DATA AND MANPOWER REQUIREMENTS

The data inputs which are required to implement REM can be divided into those which pertain to the particular location being modeled, such as gridded emission densities, and those which pertain to the operation of the model, such as the number of lines to be used in printer plot output. The latter types of inputs are not discussed here, since they are of most concern to the modeler who will operate REM. They are discussed in detail in reference 2. Details on format of the location-specific inputs are also excluded in this discussion for the same reasons.

REM uses a 25 x 26 grid element network to locate the moving air column, the fixed meteorological and air monitoring stations, and to allocate emissions. Each grid element is 2 miles on a side, although 2 kilometer squared grid elements may be used. Area source emissions for each grid element are required as direct inputs to the model for the following pollutants:

- Reactive hydrocarbons (propylene)
- "Less reactive" hydrocarbons
- Nitric oxide

Mobile source emissions are computed in the model from the following inputs:

- Emission factors for
  - Reactive hydrocarbons (propylene)
  - Less reactive hydrocarbons
  - Nitric oxide
  - Carbon monoxide
- Freeway traffic mileage for each grid element (daily totals)
- Street traffic mileage for each grid element (daily totals)

Built into REM is the temporal distribution of daily traffic for freeways and streets. The fraction of the daily traffic counts corresponding to the time of day at which the air column passes through a particular grid element is multiplied by the total daily traffic to find the VMT for that hour for that grid.

Meteorological data required as inputs to the model include, for each station as available for up to 32 stations are:

- Wind speed
- Wind direction
- Temperature
- Dew point

The model computes relative humidity internally from temperature and dew point data. Relative humidity is used in calculating the photodissociation rate constant for NO_2. Also included in this calculation are cloud type and solar angle. Cloud type must be input to the model based on the following types:

- Cirrus
- Cirrostratus

- Altocumulus
- Altostratus
- Stratocumulus
- Stratus
- Fog

The solar angle is required for each hour of the day.

The final meteorological inputs required to run REM relate to mixing height. These data may be input either as mixing heights by hour of day directly, or as the previously discussed morning and afternoon temperature soundings. In the latter case the program computes mixing heights from the soundings and surface temperature data.

As mentioned earlier, REM places most emphasis on the chemical reaction mechanisms. These must be supplied as inputs consisting of the chemical reactions and their rate constants.

The reactions and rate constants were given in Table 8. They were derived from reaction chamber data and can be used for locations other than Los Angeles, with the exception of the NO_2 photodissociation rate, which should be adjusted to other locations. The final inputs required are the initial pollutant concentrations in the air column at the beginning time and location of the trajectory.

Because of the relative simplicity in setting up the input data for REM (DIFKIN and the SAI Areawide models are discussed in the next two sections) it requires the least effort of these three models. The largest effort, which is common to all three models, is establishing the grid network and allocating the VMT and area source data to each grid element. Table 9 indicates the estimated manpower needed for this effort, based on GCA experience in Denver, Colorado. These estimates are given

as guides with the understanding that there can be variability from location to location, depending on the availability of recent traffic surveys and emissions inventories. For locations where the APRAC model has been applied, the gridding procedure and VMT allocation should be readily available. Preparation of the remaining inputs on meteorological variables and initial concentrations should take approximately 80 manhours at most, and the bulk of this time would be spent collecting the data from different sources.

Table 9. ESTIMATED MAXIMUM TIME AND COSTS FOR OBTAINING TRAFFIC AND AREA SOURCE INPUTS FOR REM

Work required	Estimated man-hours	Estimated cost[a]		
		Personnel	Computer	Total
Establish grid, code traffic links to grid	400[b]	$2,800	$800	$3,600
Determine diurnal variation in VMT	80	560	–	560
Allocate area source emissions to grid	80[c]	560	–	560
Total	560	$3,920	$800	$4,720

[a]Assumes an average rate of $7.00 per man-hour and $800 per hour of computer time.

[b]Based on experience in Denver, Colorado, for DIFKIN model.

[c]Assumes emissions are allocated homogeneously to grid elements from county-wide totals.

APPLICATION OF THE TECHNIQUE

Details on implementing REM for photochemical oxidant prediction are provided in reference 2. This reference may be consulted for full information on required data inputs and formats, while means for obtaining these inputs are discussed here.

The main effort in getting REM up and running is overlaying the grid network and allocating the area source emissions and mobile source VMT to each grid element. Obtaining these data was discussed in Sections II and III of this report. Area source emissions can be allocated to each grid according to area from county-wide emission inventory data from NEDS. The fraction of county-wide emissions (or some other geographical detail) could also be weighted into each grid element by population density. Point source emissions, which are treated as area source emissions because of the homogeneous concentration profile in the vertical direction which is assumed in the model, should be allocated directly to the grid element which the point source occupies.

VMT data, as discussed in Section II, are generally available from the local highway department or planning agency for roadway links. These data must be allocated to the individual grid elements. This almost necessitates the use of a computer because of the volume of data to be handled. Programs have been written to grid the VMT from link data, but none is generally available. Agencies which have used the APRAC model for carbon monoxide will usually have such programs available, and, if APRAC has been run recently, they may have the required VMT data in gridded form. The local highway department or planning agency should also be contacted for temporal distributions of street and freeway traffic.

Meteorological data include station locations, including elevation, wind speed and direction, temperature, dew point, and temperature soundings. Wind data may be available from local air pollution agencies, highway agencies, airports, universities, and power plants. Temperature and dew point data are usually not so readily available. The National Weather Service or local airports taking surface observations should be able to supply these data. Temperature soundings, used to compute mixing heights, are least available. The National Weather Service should be contacted to determine if these data are taken for a particular

location. REM has the option of using mixing height inputs directly. These are also available from the National Weather Service as interpolated values for many locations which do not have sounding data.

Solar zenith angle is given in the model[1,2] for Los Angeles. For other locations, Tables 169 and 170 of the Smithsonian Meteorological Tables[4] can be used to compute the angle for each hour of the day for any day of the year.

LIMITATIONS

The general application of REM in its current form is limited by its specificity to Los Angeles and by the fact that validation has been attempted only for Los Angeles. Neither of these problems is excessively severe, however. The Los Angeles specific feature which is "built-in" to the model applies to meteorological stations. The effect is to disallow the use of certain station and trajectory location combinations because of intervening mountains. This is easily changed by removing SUBROUTINE BARIER from the computer program.[2] Validation for cities other than Los Angeles could be accomplished relatively easily, compared to the DIFKIN model and the SAI Areawide model.

A limitation of REM for highway system review is its basic structure around a Lagrangian, or moving coordinate system. Since oxidant concentrations are computed only at a specific point at a desired time, or at a specific time at a desired point, the model must be run repeatedly to gather enough space and time points to assess fully VMT temporal and spatial changes.

Another limitation to REM, which can, of course, be eliminated by modifying the computer code, is its treatment of mobile source emissions. The model calls for inputs of emission factors for reactive hydrocarbons, "less reactive" hydrocarbons, nitric oxide, and carbon monoxide. The

emission factors are presumably for a mix of light-duty vehicles. There is no mention of heavy-duty vehicles either for separate factors or for inclusion in a mix with light-duty vehicles. There is no speed adjustment for emission factors, although VMT for street and freeway traffic for each grid element are required inputs to the model.

SPECIAL FEATURES

The REM model has spatial and temporal detail far in excess of any of the models considered thus far. As a trajectory model, this detail makes it suitable for the evaluation of highway project impacts on oxidant concentrations. It can also be used for system evaluation, although this is somewhat clumsy, since it requires numerous model runs to develop enough information for full assessment.

While REM is weak in its treatment of atmospheric transport and diffusion processes, it uses a detailed chemical module for explicit calculation of photochemical processes. It considers almost twice as many chemical reactions as any of the other models described in this report. However, this does not necessarily imply that its treatment depicts reality any better than DIFKIN or the SAI model.

A final feature of REM is that it is easier to apply, requiring fewer data inputs and having a simpler code, than DIFKIN or the SAI model.

REFERENCES

1. Controlled Evaluation of the Reactive Environmental Simulation Model (REM). Volume I: Final Report. Pacific Environmental Services, Inc. EPA Report EPA R4-73-013a. February 1973.

2. Controlled Evaluation of the Reactive Environmental Simulation Model (REM). Volume II: User's Guide. Pacific Environmental Services, Inc. EPA Report EPA R4-73-013b. July 1973.

3. "1969 Atmospheric Reaction Studies in the Los Angeles Basin, Volume I," Scott Research Laboratories, Final Report, Contract No. CPA 70-6.

4. Smithsonian Meteorological Tables, Publication 4014, Smithsonian Institution, Washington, D. C. 1951.

SECTION VIII

DIFFUSION KINETICS MODEL

The next level of model complexity is the Diffusion Kinetics (DIFKIN) model. As in the case of REM, DIFKIN calcuates the trajectory of an air parcel across an emission grid network and determines time dependent concentrations of reactive pollutants. Unlike REM, in DIFKIN the equation for turbulent diffusion in the vertical direction is solved to obtain concentrations and fluxes for as many as ten mesh points from the ground surface to the top of the mixing layer.

APPLICABILITY AND RELIABILITY

As a trajectory model, DIFKIN is most applicable for project level analysis. It is ideally suited to relating emissions along an air parcel trajectory to concentrations observed at later times further along the trajectory. However, it can still be used for highway system analysis, as was the case with REM, by repeated applications of the model to develop a sufficient number of trajectories for adequate spatial and temporal coverage of a region.

Although DIFKIN considers vertical diffusion of pollutants up to the mixing height, horizontal diffusion is ignored. This implies that the model is more applicable to regions with only small emission gradients between adjacent grid elements. The effect of ignoring horizontal diffusion has been investigated,[1] and under "worse case" emission gradient conditions the errors are about 40 percent. For normal operating conditions the effect is negligible.

Again, as with REM, DIFKIN calculates a trajectory along which the air parcel travels by interpolating between wind data taken at monitoring sites in the region. The greater the density of these meteorological monitoring sites the better DIFKIN will be able to replicate a "true" trajectory. Thus, in practice, DIFKIN becomes more applicable operationally as the available meteorological monitoring sites become more dense in a region.

Tests of the validity of DIFKIN have been performed in Los Angeles,[1] San Francisco,[2] and Denver.[3] For the Los Angeles case, validation was performed for the six day period in the fall of 1969 for which REM and the SAI model were also validated. Three of these days involved "hands-on" tests to vary different model parameters and calibrate the model. On the other three days the model was run "hands-off." Table 10 shows the correlation coefficients between calculated and observed ozone concentrations for the "hands-on," the "hands-off," and the composite model runs, and the regression equation for the composite.

Table 10. CORRELATION COEFFICIENTS AND REGRESSION EQUATION FOR DIFKIN IN LOS ANGELES[1]

	Hands-on	Hands-off	Composite
r	0.94	0.88	0.92
n	≈75	≈75	151

Observed ozone (pphm) = 0.840 calculated ozone (pphm)
+ 2.307 (pphm)

Standard error = 2.109 pphm

From the regression equation, it is seen that DIFKIN tends to underestimate low concentrations and to overpredict at high concentrations, with the crossover occurring at about 15 pphm of ozone.

During the validation, the emission fluxes of NO were reduced by 75 percent from the emission inventory estimates in order to gain better agreement with observed ozone concentrations. It was also found[1] that predictions of NO and NO_2 had to be sacrificed to improve the ozone correlations.

Perhaps the most significant result, which was also experienced with the Denver case,[3] was the very high sensitivity of the model predictions to the initial pollutant concentrations used to "seed" the calculations. This was found to be very important for trajectories beginning about 6:00 a.m. and running for a time less than 8 hours. A preliminary sensitivity analysis of DIFKIN has been performed by the California Division of Highways.[4] This analysis determined the percent change in predicted concentrations of O_3, NO, NO_2, and HC for a 50 percent increase in each of various model input parameters dealing with initial pollutant concentrations, chemical reaction rates, meteorological inputs, and growth and adjustment factors. The results, which are given in Table 11, show the highest sensitivity to be that of ozone to the initial concentration of hydrocarbons.

In an application for San Francisco,[2] the model worked well, with a correlation coefficient between calculated ozone and observed oxidant concentrations of 0.88 for 22 data pairs. These comparisons are for trajectory end points, and they range from noon to 5:00 p.m. The root-mean-square difference between calculated and observed or interpolated concentrations was 2.65 pphm. Although NO emissions were not reduced by 75 percent in these model runs, minor adjustments were made in 9 of the 22 trajectories. Each of the trajectories began near the coast or over the ocean. As a result, it was assumed that pollutants were uniformly mixed in the vertical direction, and that the initial concentrations were

Table 11. PERCENT CHANGE IN PREDICTED CONCENTRATIONS OF O_3, NO, NO_2, AND HC FOR A 50 PERCENT INCREASE IN EACH OF VARIOUS MODEL PARAMETERS[4]

50 percent increase in	Percent change in prediction of			
	O_3	NO	NO_2	HC
Initial concentration of:				
O_3	0	0	0	0
NO	-47	86	-1	5
NO_2	-13	14	0	1
HC	187	-66	4	18
Reaction rates:				
K_1	*	*	*	*
K_2	-24	-3	3	1
K_3	3	-3	0	-1
K_4	147	-59	3	-14
K_5	0	0	0	-1
K_6	-3	0	-1	0
K_7	-24	24	-3	3
K_8	-53	83	-13	8
K_9	3	-3	0	-4
K_{10}	0	0	0	0
K_{11}	-16	24	1	7
K_{12}	12	0	0	0
K_{13}	0	0	0	0
K_{14}	0	0	0	0
K_{15}	13	-14	0	-1
K_{16}	13	-24	-7	-1
Basic inputs:				
Mixing height	81	-39	-47	-48
Vertical mesh interval	37	-21	-3	3
Growth and adjustment factors:				
Stationary sources (all pollutants)	-42	97	13	16
Automobile growth (all pollutants)	-21	55	8	11
NO_x: Stationary	-32	45	4	1
Power plant	-24	38	4	1
Oil refinery	-13	14	1	0
Surface street	-29	45	4	1
Freeway	-18	28	3	1
HC: Stationary	21	-17	2	10
Oil refinery	5	-7	0	1
Surface street	16	-10	1	7
Freeway	3	-3	0	1
Base case concentration (pphm)[a]	3.8	2.9	15.7	13.4

* Function of sun angle.

[a] Concentration at 1700 (maximum predicted O_3 concentration) after 10-hour simulation.

1 pphm for all pollutants except CO and ozone. CO was assumed to be present at 1 ppm, while ozone was based on the relationship

$$[O_3] = \frac{k_1[NO_2]}{k_2[NO]} \quad . \tag{27}$$

A preliminary application of DIFKIN to Denver[3] yielded a correlation of 0.33 between calculated and observed concentrations for five data pairs. The DIFKIN calculated values were lower than observed ozone levels in all cases. The Denver experience also showed the predicted values to be very sensitive to the initial hydrocarbon concentrations. Additionally, it was found that the rise in calculated ozone concentrations with time was relatively insensitive to the trajectory which was followed, and hence to the emissions being input into the air parcel.

The only change made in DIFKIN for application to Denver (aside from removing mountain barriers) was to increase the photodissociation rate for the production of ozone and NO from NO_2 by 15 percent to account for the increased solar intensity due to the altitude increase. The emission fluxes of NO were used directly and not reduced by 75 percent.

DATA AND MANPOWER REQUIREMENTS

A rather extensive input data set is required by DIFKIN. Much of this involves job control parameters, while other data apply to emissions, meteorology, and the photochemical reaction scheme and rates. A user's guide to DIFKIN is available[5] which describes the required inputs in detail. An overview of the emissions, meteorological, and chemical reaction data inputs is presented here.

The emissions inputs constitute the largest volume of data necessary to operate the DIFKIN code. Most of these data are contained within the

program itself, so that the code must actually be modified when these emissions inputs are changed. The emissions are categorized by mobile and stationary source. The mobile source emission parameters, their units, and the required resolution are displayed in Table 12.

It is evident from Table 12 that the mobile source emissions are treated in much more detail than was the case with REM. Diurnal variations in traffic volumes, speed differentials for fast and slow directions of travel, and corrections for speed, cold starts, and hot starts are included.

The emissions data needed for stationary sources are given in Table 13. These include emissions from power plants and oil refineries as separate inputs. All other stationary source emissions fall into the category of "distributed emissions." Again displaying the potential to accommodate more detailed emissions inputs than REM, DIFKIN requires the hourly fraction of the total daily emissions for each of the three stationary source types.

The basic meteorological inputs to the model are hourly wind speed and direction measurements from as many stations as possible so that an air parcel trajectory can be determined. In addition, DIFKIN employs up to ten vertical mesh points at which concentrations are calculated, and at which vertical diffusivity coefficients must be assigned. The mixing height is the final meteorological input to the model. It is included for completeness, although it is not used and hence may be omitted.[5] The requirement for vertical diffusivity coefficients, the treatment of vertical diffusion, and the neglect of the mixing height show a fundamental difference in the approaches of REM and DIFKIN. REM assumes a well-defined volume of air, bounded by the ground at the bottom and the mixing height at the top, in which pollutants are well mixed. DIFKIN, on the other hand, uses up to eight vertical increments through which pollutants are diffused and concentrations are calculated.

Table 12. VEHICULAR EMISSIONS DATA REQUIRED FOR DIFKIN[5]

Parameter	Units	Resolution
Freeway VMT	kmi	Each grid square
Surface street VMT	kmi	Each grid square
Fraction of total daily freeway VMT	-	Each hour
Fraction of total daily surface street VMT	-	Each hour
Off peak average speed on freeways	mph	All hours except 6:00-10:00 a.m.
Peak traffic average speeds on freeways (slow direction)	mph	Each grid square, each hour between 6:00 a.m. and 10:00 a.m.
Peak traffic average speeds on freeways (fast direction)	mph	Each grid square, each hour between 6:00 a.m. and 10:00 a.m.
Peak traffic volume ratio on freeways (slow/fast)	-	Each grid square, each hour between 6:00 a.m. and 10:00 a.m.
Fraction of vehicle starts which are cold starts	-	In 8 time periods over 24 hours
Correction factor to account for emissions following cold starts	-	Each pollutant, 1.0 before 6:00 a.m. and after 9:20 a.m., function in 19 linear segments between 6:00 and 9:20 a.m., surface streets only
Exponent for emissions versus speed correlation	-	Each pollutant, freeways only
Hot-running emission factors	$\frac{\text{grams}}{\text{mile}}$	Each pollutant
Cold-start cycle emission factors	$\frac{\text{grams}}{\text{mile}}$	Each pollutant
Linear coefficient for emissions versus speed correlation	-	Each pollutant, freeways only

Table 13. STATIONARY SOURCE EMISSIONS DATA REQUIRED FOR DIFKIN[5]

Parameter	Units	Resolution
Power plant NO_x emissions	kg/hr	Daily average each grid square
Oil refinery NO_x emissions	kg/hr	Daily average each grid square
Oil refinery reactive HC emissions	kg/hr	Daily average each grid square
Distributed source NO_x emissions	kg/hr	Each grid square 6:00 a.m.-6:00 p.m. average
Distributed source reactive HC emissions	kg/hr	Each grid square 6:00 a.m.-6:00 p.m. average
Fraction of total daily power plant emissions	-	Each hour
Fraction of total daily oil refinery emissions	-	Each hour
Fraction of total daily distributed source emissions	-	Each hour

DIFKIN employs half as many chemical reactions as REM. The reactions, the reaction rates, and the stoichiometric coefficients, are all input to the model and are shown in Table 14. These have been standard in use except for the NO_2 photodissociation rate constant for the first reaction displayed in Table 14.

The increased data requirements of DIFKIN imply a greater effort to apply the model compared to REM. Most of this would be expended in actually understanding the code and getting the model operational, and much of this effort would be spent in revising the emission data which are maintained internally in the code. Collection of the emissions data and the gridding procedure are relatively similar to those of REM, and thus Table 9, which is actually based on experience with DIFKIN, is a reasonable guide for both models.

Table 14. PHOTOCHEMICAL REACTIONS AND RATE CONSTANTS USED IN DIFKIN

Reaction	Rate, $ppm^{-1}\ min^{-1}$
1. HV + NO2 = NO + O3	1×10^{-4}
2. NO + O3 = NO2 = O2	2.67×10^{-1}
3. O + HC = 8RO2	1×10^{-6}
4. OH + HC = 8RO2	1×10^{2} [a]
5. RO2 + NO = NO2 + 0.125*OH	1×10^{3}
6. RO2 + NO2 = PAN	2×10^{0}
7. OH + NO = HNO2	1.5×10^{1}
8. OH + NO2 = NHO3	3×10^{1}
9. O3 + HC = RO2	4×10^{-5}
10. HV + HONO = OH + NO	3.7×10^{-7}
11. NO2 + O3 = NO3 + O2	5×10^{-5}
12. NO3 + NO2 = N2O5	4.5×10^{1}
13. N2O5 = NO3 + NO2	1.4×10^{1}
14. N2O5 + H2O = 2HNO3	6.05×10^{1}
15. NO + NO2 + H2O = 2HNO2	1×10^{-5}
16. NO2 + PARTICLES = PRODUCTS	1×10^{-3}

[a] Variable dependent upon intial ratio of HC to NO_x.

Experiences with DIFKIN[2,3,6] have had total costs of implementation of approximately $25,000 to $35,000. This breaks down to roughly 10 to 15 percent for computer time and 85 to 90 percent for labor. Once the initial experience in applying DIFKIN has been gained by an organization, further applications to other locations can be made for an estimated $10,000 to $15,000.

APPLICATION OF THE TECHNIQUE

As in the previous section, an overview will be given here on applying DIFKIN. References 1 and 5 provide the detailed information needed to run the model. This discussion draws on information presented in Reference 3.

As described previously, certain programming changes are required to run DIFKIN for locations other than Los Angeles. These changes are needed largely due to the fact that much of the data which might more conveniently be read in externally are actually wired into the code itself. The following DIFKIN program modifications are required to incorporate a new data base:

- The appropriate wind station names and coordinates, compass point azimuths, and distance criteria must be inserted in "SETIN", a DIFKIN subroutine called upon to initialize the aforementioned variables.

- Subroutine BARIER, a routine which checks whether or not two given points are on the same side of each of a set of finite length, straight line barriers, in most cases must be altered to remove the effect of Los Angeles topographical features such as the San Gabriel mountains, Santa Monica mountains, and Palos Verdes hills. Interpolation of wind speed and direction measurements for trajectory calculations is not permitted between those stations located on opposite sides of a barrier.

- BLOCK DATA programs ONE through FIVE must be changed so that new mobile and stationary source emission parameters can be entered.

Emissions inputs are needed for stationary and mobile sources for CO, NO, and reactive hydrocarbons. Emissions of NO_2 are converted to NO emissions in the model by multiplying by the ratio of molecular weights, or 30/46. It is also assumed in the model that mobile source hydrocarbon emissions are composed of a reactive fraction which is about 70 percent of the total by weight. Different emission factors may be input for hot-start and cold-start emissions if these are available. If they are not both available,

emissions derived from AP-42[9] may be used in both cases. A study[10] of cold-start effects on photochemical smog has shown negligible impact.

Stationary source hydrocarbon emissions are to be input as reactive hydrocarbons. Studies in Los Angeles[7,8] classify 70 percent of stationary source hydrocarbon emissions (excluding refineries) as reactive, while 50 percent of refinery hydrocarbon emissions are designated as reactive.

In addition to the hourly wind speed and direction data, vertical diffusivity coefficients must be specified at each of the vertical mesh points. These may also be updated periodically during the simulation. Figure 8 shows the variation of diffusivity with height for different stability conditions. Stability estimates can be made using the methodology outlined in Reference 11.

The NO_2 photodissociation rate constant is another parameter which can be revised periodically. This is important since it is a function of the solar zenith angle. A separate program to compute this rate constant as a function of time of day is provided in Reference 5. The computed values are then input directly into DIFKIN.

In all three applications of the DIFKIN model[1,2,3] essentially the same reactions, rate constants, and stoichiometric coefficients were used, with the exception of the NO_2 photodissociation rate constant. No real guidance is offered in the user's manual as to when or in what manner different values might be used. In addition, although the model is admittedly quite sensitive to the initial concentrations inputs, no guidelines are given for choosing reasonable "seed" values, either in terms of actual concentrations or in terms of concentrations compatible with accurate predictions.

LIMITATIONS

Like REM, DIFKIN is a trajectory model, and hence it has the same limitations for highway system evaluation as were discussed for REM. The model

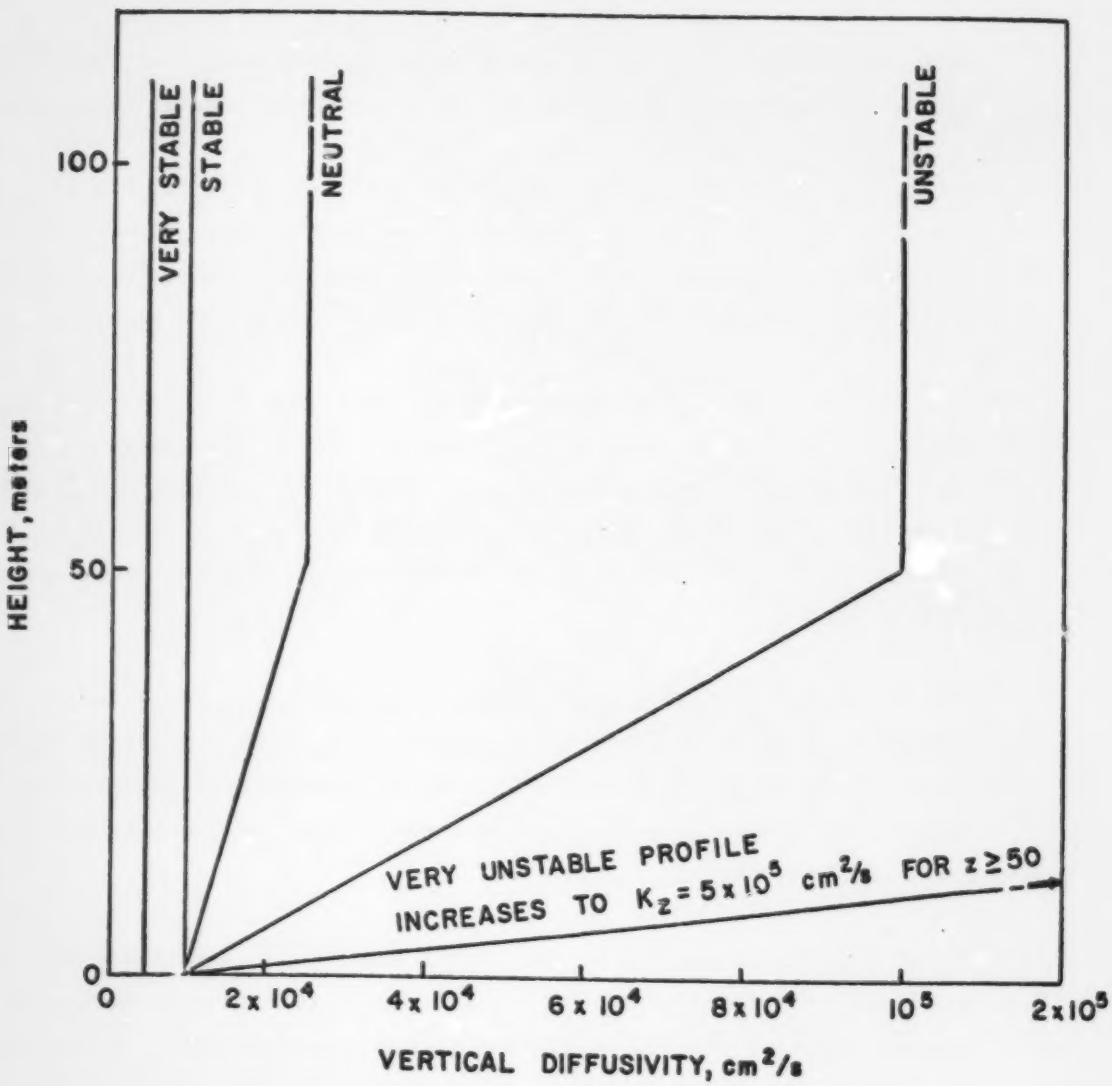

Figure 8. Variation of diffusivity with height for different stability conditions

must be run repeatedly to gather enough space and time points to assess VMT and emissions temporal and spatial changes fully. The SAI model discussed in Section IX has relatively long running times (about 1 hour of computer time for a 10 hour simulation). DIFKIN requires about 2 minutes of computer time for each trajectory. Thus, DIFKIN is not necessarily any more economical to run for system evaluation, especially considering that the individual trajectory calculations must be compiled into an overall mapping of concentrations. This operation is intrinsic to the SAI model.

The inclusion of emissions data in a "BLOCK DATA" statement within the program itself is somewhat clumsy operationally. While this is not a serious limitation to the model, it would be simpler if these data could be read in as inputs. Another problem, not especially serious, is the specificity of the model in its present form to Los Angeles topography. Mountain barriers are included in the program which exclude the use of certain combinations of meteorological station geographical locations in computing trajectories.

A more serious problem is the sensitivity of the model to initial pollutant concentrations, and the fact that this is not even acknowledged in the user's manual to DIFKIN. More guidance on the magnitude of this problem and how it might best be handled is needed.

Neglect of horizontal diffusion has been investigated[1,12] and introduces only small errors in predicted values. Under most conditions the errors are smaller than 10 percent and can generally be ignored.[12] Under extreme emission density gradients the errors may approach 40 percent.[1] DIFKIN also ignores vertical advection, and this can cause errors of a factor of two under common urban conditions.[12] Finally, neglect of vertical wind shear, inherent to trajectory models, may introduce errors of overprediction of 50 percent or greater.[12]

SPECIAL FEATURES

Many of DIFKIN's limitations are also its strengths compared to previous mod ls which have been discussed. It offers the most comprehensive treatment of atmospheric transport, diffusion, and photochemical reaction processes of any of the models described thus far. While the chemical reaction scheme is not so elaborate as that of REM, DIFKIN predicts ozone concentrations more nearly accurately. Perhaps this reflects the current state of understanding of atmospheric transport and diffusion compared to photochemistry occurring in the atmosphere.

As a trajectory model, it is well suited to determining the effects of specific sources (project level analysis) on resulting downwind concentrations. This could be a valuable tool for investigating the existence of "hot spots."

The best feature of DIFKIN might be the fact that it has been applied in a number of locations[1,2,3] and undergone other investigation.[3,4,12] Thus, many of the strengths and weaknesses of the model have been uncovered, and there exists a body of knowledge available to guide its future application.

REFERENCES

1. Eschenroeder, A. Q., J. R. Martinez, and R. A. Nordsiek. Evaluation of a Diffusion Model for Photochemical Smog Simulation. Final Report. Prepared for U.S. Environmental Protection Agency, Contract No. 68-02-0336. General Research Corp., Santa Barbara, California. 1972. 212 pp.

2. Ludwig, F. L. and J. H. S. Kealoha. Present and Prospective San Francisco Bay Area Air Quality. SRI Project 3274. Stanford Research Institute. December 1974.

3. Photochemical Oxidant Modeling: Detailed Technical Report. Final Final Report - Volume II. Report No. GCA-TR-11-G(2). GCA/ Technology Division. July 1975.

4. Ranzieri, A. J., P. D. Allen, and W. B. Crews. A DIFKIN Sensitivity Analysis for Transportation Air Quality Studies. Draft Report. California Division of Highways. 1974.

5. Martinez, J. R., R. A. Nordseick, and M. A. Hirschberg. User's Guide to Diffusion/Kinetics (DIFKIN) Code. Final Report. Prepared for U.S. Environmental Protection Agency, Contract No. 68-02-0336. General Research Corp., Santa Barbara, California. 1973. 240 pp.

6. Ludwig, F. L. Personal communication.

7. Roberts, P. J. W., et al. Extensions and Modifications of a Contaminant Emissions Model and Inventory for Los Angeles. Report No. R73-15, Prepared for U.S. Environmental Protection Agency, Contract No. 68-02-0339. Systems Applications, Inc., Beverly Hills, California. 1973. 52 pp.

8. Roberts, P. J. W., P. M. Roth, and C. L. Nelson. Contaminant Emissions in the Los Angeles Basin - Their Sources, Rates and Distribution. Appendix A of Development of a Simulation Model for Estimating Ground Level Concentrations of Photochemical Pollutants. Report No. 71SAI-6, Prepared for U.S. Environmental Protection Agency, Contract No. CPA 70-148. Systems Applications, Inc., Beverly Hills, California. 1971. 86 pp.

9. Compilation of Air Pollutant Emission Factors. Second Edition. U.S. Environmental Protection Agency. Office of Air and Water Programs, Office of Air Quality Planning and Standards, Research Triangle Park, North Carolina 27711. April 1973.

10. Martinez, J. R., R. A. Nordsieck, and A. Q. Eschenroeder. Morning Vehicle-Start Effects on Photochemical Smog. Environ Sci Technol. 7:10, October 1973.

11. Turner, D. Bruce. Workbook of Atmospheric Dispersion Estimates. U.S. Environmental Protection Agency, Report AP-26. 1970.

12. Systems Applications, Inc. Development of a Second Generation of Photochemical Air Quality Simulation Models. Progress Report. Prepared for U.S. Environmental Protection Agency, Contract No. 68-02-1237. 1974.

SECTION IX

URBAN AIR SHED PHOTOCHEMICAL SIMULATION MODEL

APPLICABILITY AND RELIABILITY

This model, which was developed by Systems Applications Inc. (SAI), provides the most detailed treatment of the physical and chemical processes important in the formation of photochemical smog of all the models studied. Concentrations of reactive species are determined by means of a finite difference scheme for an array of grid elements. Meteorological inputs to the program consist of wind speed and direction for a number of stations in a study area. These values are then interpolated to give a flow vector for each ground level grid element. Each grid element is also assigned an hourly mixing depth which depends upon the terrain elevation and the measured mixing depth at one or more meteorological stations. The input of initial concentrations and hourly meteorological variables for specified measurement locations is handled by means of data preparation programs. These programs also determine correlations between corresponding input parameters at various stations so that measured values may be extended over the entire grid system.

As part of these data preparation programs, the SAI model also employs a rather sophisticated emission inventory routine for mobile and stationary sources. In addition to standard inputs such as vehicle miles traveled (VMT) for different road types, the emissions submodel requires such detailed information as airport emissions for different aircraft types, mole fraction of NO in auto NO_x emissions, and correction factors for each pollutant species to account for the nonuniform distribution of vehicle starts.

The SAI model predicts pollutant concentrations for all grid elements in a 25 by 25 element array at discrete times. This capability makes it ideally suited for highway system evaluation among it, REM, and DIFKIN. Like REM and DIFKIN, the SAI model contains features which are specific to Los Angeles, some of which make application to other locations slightly more difficult than for the other two models.

The SAI model has been validated for the same six days in 1969 in Los Angeles for which tests were made of REM and DIFKIN. One report of this validation[1] compared calculated and observed ozone concentrations for the SAI model on two different data sets. The first was composed of data from monitoring locations. These data were used in the evaluation of REM. The second set was made up of data at trajectory points used in the DIFKIN evaluation. These did not necessarily coincide with station locations. Using the first set of data, the SAI model produced a correlation coefficient of 0.60, while REM yielded 0.50. For the second data set, the correlation coefficient was 0.69 for the SAI model compared to 0.91 for DIFKIN. Further analysis of the SAI model results showed that it tended to underpredict the station values while tending to overpredict the trajectory values, although not strictly so in either case. REM and DIFKIN exhibited these same tendencies, respectively.

DATA AND MANPOWER REQUIREMENTS

The user's manual[2,3] for the SAI model provides exhaustive explanations of data requirements and operating procedures for the model. Again, this should be consulted for detailed information. The following description of the data requirements and outputs is intended to provide an overview for comparison with the requirements of other models.

The Urban Air Shed Photochemical Simulation Model is made up of four computer programs: (1) the Atmospheric Pollution Simulation Program, (2) the Emissions Data Preparation Program, (3) the Meteorological Data Preparation

Program, and (4) the Data Plotting Program. The heart of the SAI model is the Atmospheric Pollution Simulation Program (APSP). This program accepts the input data supplied by the two data preparation programs and performs the actual pollutant concentration calculations. The Data Plotting Program is a useful accessory which plots calculated and observed concentrations as a function of time at specified locations.

The Emissions Data Preparation Program requires the following information to develop inputs to APSP:

- Automotive emissions
  - Daily miles driven on all streets (excluding freeways) in each grid square.
  - Daily miles driven on freeways in each grid square.
  - Hot and cold start emissions factors.
  - Fraction of vehicles cold started.
  - Correction factor for the nonuniform distribution of trip starts.
  - Freeway driving speeds in the fast and slow directions.
  - Emissions - driving speed correction factors.
  - Ratio of freeway vehicle miles driven in the slow direction to the number driven in the fast direction.
  - Temporal distributions of freeway and nonfreeway traffic activity.
- Aircraft emissions (ground operations)
  - Number of daily aircraft flights at each airport.
  - Temporal distribution of aircraft activity.
  - Emissions/aircraft engine.
  - Number of aircraft engines/aircraft.

- Fixed source emissions (ground-based)

  - Total distributed fixed source emissions from each grid square.

As output, this program creates a data file for use by APSP, and a print-out of the emission fluxes by hour.

The Meteorological Data Preparation Program uses hourly data on the following parameters to prepare inputs to APSP:

- Wind speeds
- Wind directions
- Mixing depths

The data file which is created as output from this program provides data on wind speeds, wind directions, the time rate of change of the mixing depths, and the time interval for which these data are applicable.

As mentioned previously, the actual concentration calculations are done by APSP. Meteorological inputs and ground level emissions inputs are accepted from the data preparation programs. In addition, the following inputs are required:

- Grid characteristics, including number of vertical strata, horizontal grid spacings, and shape of the region.
- Starting and stopping time of the simulation.
- Time interval between instantaneous concentration printouts.
- Location of monitoring stations.
- Rate, location, and temporal variation of major elevated point source emissions.
- Parameters applying to the operation of the finite differing scheme.
- Parameters applying to the chemical reaction scheme.

- Initial conditions
- Concentrations aloft
- Boundary concentrations at points of horizontal inflow

As output, APSP provides the following information:

- Printed hourly-averaged ground level concentration maps and a printed summary of the hourly-averaged concentrations predicted at each monitoring station.
- Printed instantaneous ground level concentration maps and a printed summary of the instantaneous vertical concentration distribution above each monitoring station.
- Punched cards for input to the Data Plotting Program containing the hourly-averaged concentrations predicted at each monitoring station.

The emissions data requirements of the SAI model are similar to those of DIFKIN, while the meteorological inputs are like those of REM. The efforts involved in preparing the data to run the model are thus of the order of the efforts described for these other two models. The major extra effort to employing the SAI model involves actually getting the program operational and validating it for a location other than Los Angeles. To date, only SAI has attempted to use the model outside of Los Angeles, and such attempts have not yet come to fruition. Based on experience applying the DIFKIN model in Denver,[4] and the much longer running time of the SAI model, it is estimated that as much as an additional $10,000 above the DIFKIN efforts might be required for initial implementation of the model.

APPLICATION OF THE TECHNIQUE

Ample information on the methodology and operation of the various programs in the SAI model is given in References 2, 3, 5. These must be consulted for any detailed information. General information on emissions data is given in previous sections of this report. Methods for developing the meteorological data are described in Section VII.

Data on the frequency of operation of different aircraft categories are required for the emissions program of this model. These may be taken from AP-42.[6]

This model calculates vertical diffusion coefficients internally as a function of wind speed and height. The horizontal diffusion coefficient is fixed. On the other hand, the NO_2 photodissociation rate change during the day is handled by inputting fractional values of the nominal, input rate constant for each hour.

As with REM and DIFKIN, mountain barriers must be removed from the program, or changed, to allow full use of the wind data. In addition, the SAI model divides the Los Angeles region into different subregions to be used in interpolating between air quality monitoring stations and specifying initial concentrations for each grid cell, in performing a similar function for wind speed and direction, in specifying mixing depths based on inversion height and general features of the underlying terrain, and in estimating concentrations at the boundary of the region. These subregions are built into the program and must be removed or modified to fit other locations.

LIMITATIONS

Perhaps the greatest limitations to the use of the SAI model are its complexity and expense. These limitations detract from its applicability to general use both in getting the model operational in a new location and in making successive runs once the model is actually functioning. A simulation for one "day" (10 hours of daylight) requires over an hour of computation time on an IBM 370/155 computer. This makes the model much more expensive to implement initially than REM or DIFKIN. The cost of getting similar amounts of information does not differ so much among the models, however, because multiple trajectories must be run for DIFKIN and REM.

The initial application of the model to any given location is made difficult by the fact that some aspects of the program are quite specific to Los Angeles. In particular, for the correlation of wind speeds, wind directions, and mixing depths, the Los Angeles basin is subdivided within the program itself into a number of topographically similar regions. Another drawback to the application of the SAI model from the viewpoint of a potential user is the inability to specify different values of horizontal and vertical diffusion coefficients without making modifications to the program itself. This situation seems curious in light of the significant role played by these variables in the determination of ozone of NO_x concentrations and the extensive amounts of computer time required for the simulation of these diffusion effects.

Although there are plans to implement the model in a number of cities, under the sponsorship of the U.S. DOT, the model has been run for Los Angeles only thus far, and only SAI has had experience with its use. This has limited the development of experience and knowledge of its capabilities. Two recent studies[4,7] have chosen to use DIFKIN over the SAI model, partly due to its expense. One of these studies[4] concluded that in spite of the fact that the SAI model is an excellent research tool, the long running times and extensive data requirements make it difficult to use the model for analysis of different transportation strategies without a considerable investment in time and manpower.

One other limitation to the SAI model involves the finite differencing scheme used to solve the atmospheric diffusion equation for this Eulerian, fixed-grid type model. Intrinsic to these models is the production of numerical or "pseudo" diffusion of material between grid cells due to the finite difference approximation to the solution of the diffusion equation. The effect in the SAI model is to introduce a harmonic error which is amplified with time, and which approaches 50 percent after a 9-hour simulation.[1]

SPECIAL FEATURES

The most important advantage of the SAI model over the other two complex computer models investigated is its ability to predict concentrations for all grid squares at a particular time. This feature makes it especially well suited to highway system evaluation.

The SAI model treats the atmospheric transport and diffusion process in more detail than any other model. It also uses the most complete emissions data set. The capacity to accommodate different topological features and boundary concentrations, while increasing the difficulty of implementation, attempts to replicate real-world processes more closely than the other models.

REFERENCES

1. Systems Applications, Inc. Development of a Second Generation of Photochemical Air Quality Simulation Models. Progress Report Prepared for U.S. Environmental Protection Agency, Contract No. 68-02-1237. 1974.

2. Reynolds, S. D. Urban Air Shed Photochemical Simulation Model Study: Volume II - User's Guide and Description of Computer Programs. Systems Applications, Inc. U.S. Environmental Protection Agency, Publication No. EPA-R4-73-030f. July 1973.

3. Whitney, D. Urban Air Shed Photochemical Simulation Model Study: Volume II - User's Guide and Description of Computer Programs: Appendix - Data Preparation Programs. Systems Applications, Inc. U.S. Environmental Protection Agency, Publication No. EPA-R4-73-030g. July 1973.

4. Photochemical Oxidant Modeling: Detailed Technical Report. Draft Final Report, Volume II. GCA/Technology Division. GCA-TR-75-11-G(2). April 1975.

5. Reynolds, S. D., Mei-Kao Lui, T. A. Hecht, P. M. Roth, and J. H. Seinfield. Urban Air Shed Photochemical Simulation Model Study. Volume I - Development and Evaluation (With Appendices). Systems Applications, Inc., Beverly Hills, California. Prepared for Office of Research and Development, U.S. Environmental Protection Agency, Washington, D.C. EPA-R4-73-020a-e. July 1973.

SPECIAL FEATURES

The most important advantage of the SAI model over the other two complex computer models investigated is its ability to predict concentrations for all grid squares at a particular time. This feature makes it especially well suited to highway system evaluation.

The SAI model treats the atmospheric transport and diffusion process in more detail than any other model. It also uses the most complete emissions data set. The capacity to accommodate different topological features and boundary concentrations, while increasing the difficulty of implementation, attempts to replicate real-world processes more closely than the other models.

REFERENCES

1. Systems Applications, Inc. Development of a Second Generation of Photochemical Air Quality Simulation Models. Progress Report Prepared for U.S. Environmental Protection Agency, Contract No. 68-02-1237. 1974.

2. Reynolds, S. D. Urban Air Shed Photochemical Simulation Model Study: Volume II - User's Guide and Description of Computer Programs. Systems Applications, Inc. U.S. Environmental Protection Agency, Publication No. EPA-R4-73-030f. July 1973.

3. Whitney, D. Urban Air Shed Photochemical Simulation Model Study: Volume II - User's Guide and Description of Computer Programs: Appendix - Data Preparation Programs. Systems Applications, Inc. U.S. Environmental Protection Agency, Publication No. EPA-R4-73-030g. July 1973.

4. Photochemical Oxidant Modeling: Detailed Technical Report. Draft Final Report, Volume II. GCA/Technology Division. GCA-TR-75-11-G(2). April 1975.

5. Reynolds, S. D., Mei-Kao Lui, T. A. Hecht, P. M. Roth, and J. H. Seinfield. Urban Air Shed Photochemical Simulation Model Study. Volume I - Development and Evaluation (With Appendices). Systems Applications, Inc., Beverly Hills, California. Prepared for Office of Research and Development, U.S. Environmental Protection Agency, Washington, D.C. EPA-R4-73-020a-e. July 1973.

6. Compilation of Air Pollutant Emission Factors. Second Edition. U.S. Environmental Protection Agency, Office of Air and Water Programs, Office of Air Quality Planning and Standards, Research Triangle Park, North Carolina 27711. April 1973.

7. Ludwig, F. L. and J. H. S. Kealoha. Present and Prospective San Francisco Bay Area Air Quality. SRI Project 3274. Stanford Research Institute. December 1974.

ENVIRONMENTAL PROTECTION AGENCY
Technical Publications Branch
Office of Administration
Research Triangle Park, North Carolina 27711

OFFICIAL BUSINESS

AN EQUAL OPPORTUNITY EMPLOYER

POSTAGE AND FEES PAID
ENVIRONMENTAL PROTECTION AGENCY
EPA - 335

U.S. MAIL

Return this sheet if you do NOT wish to receive this material ☐, or if change of address is needed ☐. (Indicate change, including ZIP code.)

PUBLICATION NO. EPA-450/3-75-069-a